NISTIR 7303

Intercomparison Program for Organic Speciation in PM2.5 Air Particulate Matter: Description and Results for Trial III

Michele Schantz, Dianne Poster,
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NIST
National Institute of Standards and Technology
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Michele Schantz, Dianne Poster, John Kucklick*, and Stephen A. Wise
Analytical Chemistry Division
National Institute of Standards and Technology
Gaithersburg, MD 20899-8392 and *Charleson, SC 29412-9110

Stephen McDow
Human Exposure and Atmospheric Sciences Division
US Environmental Protection Agency
Research Triangle Park, NC 27709

Joellen Lewtas
Human Exposure and Atmospheric Sciences Division
US Environmental Protection Agency
Seattle, WA 98101
Current Address:
Dept. Environmental and Occupational Health Sciences
University of Washington
Seattle, WA 98195

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Abstract

A working group of investigators, who are characterizing and quantifying the organic compounds in particulate matter (PM) as part of the US Environmental Protection Agency's (EPA's) PM 2.5 research program and related studies, was established to advance the quality and comparability of data on the organic composition of PM. This group has completed its third interlaboratory comparison study. The third study included two parts: Trial IIIa and Trial IIIb. Participants in Trial IIIa received a sample of SRM 1648 Urban Particulate Matter and a sample of PM2.5 collected recently in Baltimore, MD along with a sample of SRM 1649a Urban Dust. The participants in Trial IIIb received four filters of RM 8785 Air Particulate Matter on Filter Media along with a sample of SRM 1649a. The target analytes for these comparison studies include polycyclic aromatic hydrocarbons (PAHs), nitrated PAHs, alkanes (including hopanes and cholestanes), sterols, carbonyl compounds (ketones and aldehydes), acids (alkanoic and resin), phenols, and sugars. Because this is a performance-based study, laboratories are encouraged to use the methods that they are routinely using in their laboratories to analyze similar samples. The consensus values, accuracy and precision assessments, and the methods used by each laboratory are summarized in this report for Trials IIIa and IIIb.

Introduction

Organic chemicals adsorbed to fine particulate matter (PM) in the ambient air account for a major component of the PM mass and include source tracers as well as toxic compounds that may contribute to adverse human health effects. A working group of PM investigators from the US Environmental Protection Agency (EPA) Supersites and related research programs was established to improve the quality and comparability of data on the organic composition of aerosols. The working group is known as the PM2.5 Organic Speciation Working Group and includes researchers involved in the EPA PM Supersites and related sites, EPA PM Research Centers, national laboratories and other research centers, as well as regional and state laboratories. The goal of the working group is to improve the characterization and quantification of organic compounds associated with fine PM through participation in interlaboratory comparison exercises and to provide input for the development of appropriate Standard Reference Materials (SRMs). Improvements in the quality of organic measurements will allow the comparison of organic species across geographic regions and will aid in source receptor modeling, in relating toxicity and health outcomes to specific organic species, and in assessing human exposure to specific organic species and sources.

To aid in this effort, the National Institute of Standards and Technology (NIST) is coordinating a series of interlaboratory trials using PM samples through the Intercomparison Exercise Program for Organic Contaminants in PM2.5 Air Particulate Matter. The initial interlaboratory trial utilized PM from a bulk portion of Standard Reference Material (SRM) 1649a Urban Dust, which had been sieved to less than 63 μm, and an extract of these particles. The original SRM 1649, collected in Washington, DC and issued in 1982, was reissued as SRM 1649a in 2000. SRM 1649 and SRM 1649a were sieved to less than 123 μm when prepared. The second interlaboratory trial utilized a PM2.5 (2.5 μm, aerodynamic diameter) sample collected in Baltimore MD. Results from the first two trials are summarized in NISTIR 7229 [1]. Trial III included three samples, SRM 1648 Urban Particulate Matter, a second PM2.5 sample collected in Baltimore, MD, and RM 8785 Air Particulate Matter on Filter Media (A Fine Fraction of SRM 1649a Urban Dust on Quartz-Fiber Filters) with SRM 1649a used as a control sample. Results from these trials will provide the basis for improved quality assurance (QA) measures and methods for characterizing the PM-associated organic matter. The target organic analytes vary among the participants and include: alkanes (including hopanes and cholestanes), alkenes, aromatic and polycyclic aromatic hydrocarbons (PAHs), nitrated PAHs, sterols, carbonyl compounds (e.g., ketones and aldehydes), acids (alkanoic and resin acids), phenols, methoxyphenols, and sugars. The participating laboratories are not constrained by a specific analytical method; however, the laboratories are requested to summarize the methods used so that the results from different methods can be compared.

The third interlaboratory comparison study (Trial III) was initiated in August 2004. The third study included two parts: Trial IIIa and Trial IIIb. Participants in Trial IIIa received a sample of SRM 1648 Urban Particulate Matter and a sample of PM2.5 collected recently in Baltimore, MD along with a sample of SRM 1649a Urban Dust. The participants in Trial IIIb received four filters of RM 8785 Air Particulate Matter on Filter Media along with a sample of SRM 1649a.

Participants could choose to participate in one or both parts. A brief discussion of percent differences among the 10 laboratories who had reported results for Trial III by February 2005 was held at the Organic Speciation Working Group meeting convened during the American Association for Aerosol Research (AAAR) Supersite Conference in February 2005 in Atlanta, GA. Since then, an additional four laboratories have reported data for Trial III. The Trial III results and summary statistics for all of the laboratories reporting results to date are detailed in this report.

Sources and Preparation of Materials used in Intercomparison Trial III

SRM 1649a has been used as a control sample for all three trials. The original SRM 1649 (currently available as SRM 1649a) was collected in the Washington, DC area in the late 1970s over a period in excess of 12 months using a baghouse. The material was removed from the baghouse filter bags and combined in a single lot. The lot was passed through a 125 μm sieve. The sieved material was mixed in a V-blender. SRM 1649a was rebottled (500 mg per bottle), and each participant received one bottle.

Trial IIIa. SRM 1648 Urban Particulate Matter was collected using a baghouse in the mid 1970s in St. Louis, MO. The material was removed from the baghouse filter bags and combined in a single lot. The lot was passed through a 53 μm sieve. The sieved material was mixed in a V-blender. Some of the bulk air particulate was bottled (500 mg per bottle) and labeled as SRM 1648. Each participant received one bottle.

The PM2.5 material was collected in the city of Baltimore, MD at the location of the primary sampling site for the Baltimore PM Supersite [2] in the vicinity of major Baltimore industries, e.g., incinerators and factories to the south and southwest and also several major highways to the west and east. The material was collected from September 2002 to November 2002. The sampling apparatus was an Ultra-High-Volume Sampler (UHVS), consisting of an air inlet, cyclone separator, filter cassettes, and a regenerative blower. The fine particles (2.5 μm, aerodynamic diameter) were separated in the high-volume aluminum cyclone sampler and collected onto an array of Teflon membrane filters. At the end of each collection, the filters were exchanged in a trailer with temperature and humidity control. The loaded filters were brought back to NIST where the air particulate was brushed off the filter inside a plexiglass glove box. The total amount of air particulate collected for use as the Baltimore-2 PM was 12.5 g. This material was placed in a 100 mL glass bottle and mixed for 3 h on a bottle roller. The material was then aliquoted into approximately 100 mg portions in amber bottles with Teflon-lined lids. A total of 65 bottles of Baltimore-2 PM were prepared. With the use of the aluminum cyclone, the iron content of the Baltimore-2 PM was approximately 23 times lower [3] than that of the PM 2.5 Interim Reference Material used for Trial II [1]. One bottle of Baltimore-2 PM (approximately 500 mg) was sent to each of the laboratories participating in Trial IIIa. The instructions and data sheet that accompanied the samples are provided in Appendix A. In the letter accompanying each shipment, each participant was asked to analyze each of three replicate samples and to concurrently analyze the NIST SRM 1649a, Urban Dust.

Trial IIIb. Four filters of RM 8785 Air Particulate on Filter Media plus one blank filter were sent to each participant in Trial IIIb. RM 8785 was prepared by resuspending SRM 1649a in air and collecting the aerosol on quartz-fiber filters. Each filter was housed in a filter pack designed to pass only particles nominally <2.5 μm. The mass of PM on each filter is known, and this information was provided to the participants. Four filters of RM 8785, one blank filter, and one bottle of SRM 1649a (approximately 500 mg) were sent to each of the laboratories participating in Trial IIIb. The instructions and data sheet that accompanied the samples are provided in Appendix A. In the letter accompanying each shipment, each participant was asked to analyze each of three filters containing PM and the blank filter and to concurrently analyze the NIST SRM 1649a Urban Dust.

Evaluation of Exercise Results

Establishment of the Assigned Values

The following guidelines were used by the NIST exercise coordinators for the establishment of the exercise assigned values for these exercises. The laboratory's performance on concurrent reference material (SRM 1649a) analyses was used to determine if that laboratory's results would be included in the calculation of the exercise assigned value for the unknown material for a particular analyte. The results reported for the unknown materials from laboratories that did not report results for the reference material were not used in these calculations. After the exercise assigned values, standard deviations, and 95% confidence limits had been calculated, all reported results for the SRM 1648, Baltimore-2 PM, and RM 8785 materials were evaluated relative to these exercise assigned values.

Laboratory data submission: Each participating laboratory was asked to submit data from three replicate determinations of the unknown materials (SRM 1648, Baltimore-2 PM, and RM 8785) and was requested to report results of concurrent analyses of NIST SRM 1649a. Laboratories were requested to report these results to three significant figures and to provide brief descriptions of their extraction, cleanup, and analytical procedures.

Determination of laboratory analyte means: For each laboratory, the laboratory analyte mean of the three sample results (S1, S2, and S3) was calculated for each analyte. Non-numerical data were treated as follows: A mean "<value" was used when three "<values" were reported; NA (not analyzed/determined) was used for three reported NAs, etc.; and, if the reported results were of mixed type, e.g., S1 and S2 were numerical values and S3 was reported as "<value", the two similar "types" were used to either determine the mean or to set a non-numerical descriptor.

Determination of assigned values: For a particular analyte, the performance on the reference material (SRM 1649a) was deemed acceptable for the purpose of this study if the laboratory result was within 30% of the upper and lower limits of the confidence interval for analytes listed as certified or reference values in the Certificate of Analysis for SRM 1649a. For each analyte of interest not listed as a certified or reference value in SRM 1649a, no target concentration was used. If a laboratory demonstrated acceptable performance on a particular analyte in the reference material, the laboratory's results for that analyte in the corresponding "unknown"

exercise material were then used in the calculation of the analyte's exercise assigned value unless the mean was deemed an outlier. For evaluation of potential outliers, statistical tests and expert analyst judgement were used after viewing both normal and log plots of the data. This judgement utilized knowledge of potential coeluters based on the laboratory's reported methods.

Reported Results

Laboratories were assigned numerical identification codes in order of receipt of data for Trial III with the exception of NIST which is Laboratory 1 in these exercises. There are three sets of NIST results included (1a, 1b, and 1c). A laboratory was assigned the same code for each material. A list of participating laboratories in alphabetical order is given in Appendix E. In this report, the laboratory mean replicate data are shown in Tables 1, 2, 3, and 4 for SRM 1648, Baltimore-2 PM, RM 8785, and SRM 1649a reported with Trial III, respectively. Included in these tables are the exercise assigned values, the standard deviation of the assigned value, and the percent relative standard deviation (% RSD). Notes included by a laboratory with its data are listed in Appendix B. Summaries of the methods used by each laboratory are in Appendix C.

In Appendix D, charts of the mean reported numerical results by laboratory for each analyte for which more than two laboratories reported data are shown for the exercise material and the corresponding reference material. In this appendix, the data for each analyte are presented in each material (SRM 1648, Baltimore-2 PM, and RM 8785 with the corresponding data for SRM 1649a on the same page) followed by the next analyte so that the reader can compare results for each analyte in the three samples.

Performance Scores

The exercise coordinators recognize that different programs have different data quality needs. The acceptability of the results submitted by a particular laboratory will be decided by the individual program(s) for which the particular laboratory provides data. Typically, the program will use these exercise results in conjunction with the laboratory's performance in the analysis of certified reference materials and/or control materials, and of other quality assurance samples. These exercise results are shown in a number of ways in this report to facilitate their use by these programs in their acceptability assessments.

The International Union of Pure and Applied Chemistry (IUPAC) guidelines [4] describe the use of z-scores and p-scores for assessment of accuracy and precision in intercomparison exercises such as those described in this report. These indices assess the difference between the result of the laboratory and the exercise assigned value and can be used, with caution, to compare performance on different analytes and on different materials.

Accuracy Assessment (z-score)

The z-score is a bias estimate divided by a performance criterion so that $z = (x - X)/\sigma$ where x is the individual laboratory result, X is the exercise assigned value, and σ is the target value for standard deviation. As described in the IUPAC guidelines, the choice of σ is dependent upon

data quality objectives of a particular program. It can be fixed and arrived at by perception, prescription, or reference to validated methodology (e.g., $\sigma = 0.025$ X, where X is the analyte concentration), or it can be an estimate of the actual variation (e.g., the calculated standard deviation, s, from the exercise data). The fixed performance criterion is more useful in the comparison of a laboratory's performance on different materials while the use of the actual variation may be more useful within a given exercise, for example, if the determination of a particular analyte is more problematic than usual.

We have calculated and reported z-scores using both approaches for each analyte for each laboratory. At a previous workshop, it was decided to use 25% of the exercise assigned value as the fixed target value for standard deviation for this program, at least for the initial exercises. We also calculated z-scores based on one assigned-value standard deviation, s. The z-scores calculated for these exercises can thus be interpreted as shown in the following examples:

z-score (25% X):

+1	laboratory result is 25 % higher than the assigned value
-2	laboratory result is 50 % lower than the assigned value

z-score (s):

+1	laboratory result is one exercise standard deviation higher than the assigned value
-2	laboratory result is two exercise standard deviations lower than the assigned value

From a scientific point of view, IUPAC does not recommend the classification of z-scores but allows that it is possible to classify scores, e.g.:

$\|z\| \leq 2$	Satisfactory
$2 < \|z\| < 3$	Questionable
$\|z\| \geq 3$	Unsatisfactory

Tables 5 and 6 show the z-scores using 25 % and s, respectively, for the results reported by each laboratory in the Trial III samples.

Precision Assessment (p-score)

The p-score is defined as an individual laboratory's coefficient of variation (relative standard deviation for three measurements) divided by a target coefficient of variation (CV). Participating laboratories analyzed the three replicate samples for an exercise with the same sample set, i.e., one set of samples with the same blank, calibration curve, etc. applicable for each. Since the repeatability for replicates within a set is generally better than for replicates in different sets, this does not result in data that are very useful for precision (repeatability) assessment. For the calculation of p-scores for this program, the current target CV for the three replicates is 15% so a

p-score of 1 indicates that the laboratory's CV for the three subsamples was 15%. Table 7 shows the calculated p-scores for each laboratory for each reported analyte in Trial III.

Discussion

Trial III data

Laboratories were requested to quantify a wide variety of analytes in Trial III (See Table 1 in Appendix A). Twenty laboratories received the samples for Trial IIIa while twenty three laboratories received the samples for Trial IIIb. Fifteen laboratories submitted data for Trial IIIa and fourteen laboratories submitted data for Trial IIIb with the most extensive data set for the PAHs. The exercise coordinator made no changes to the data submitted.

As part of Trial III, NIST made several solutions available to those laboratories requesting them for use in the study. The solutions made available were:

SRM 2260a	Aromatic Hydrocarbons in Toluene
SRM 1491a	Methyl-Substituted Polycyclic Aromatic Hydrocarbons in Toluene
SRM 1494	Aliphatic Hydrocarbons in 2,2,4-Trimethylpentane
Candidate SRM 2264	Nitro-PAHs I in Methylene Chloride
Candidate SRM 2265	Nitro-PAHs II in Methylene Chloride
Candidate SRM 2266	Hopanes and Steranes in 2,2,4-Trimethylpentane
Candidate SRM 2267	Deuterated Levoglucosan in Ethyl Acetate
Candidate SRM 2268	Carbon-13 Labeled Levoglucosan in Ethyl Acetate

A total of 22 laboratories requested SRM 2260a, 19 requested SRM 1491a, 19 requested SRM 1494, 8 requested SRM 2267, and 7 requested SRM 2268. These were sent to the laboratories with the Trial IIIa and Trial IIIb samples. The remaining three solutions (SRM 2264, SRM 2265, and SRM 2266) were made available after the participants had the Trial III samples. Only three laboratories requested each of these three solutions.

The exercise assigned values and standard deviations for the samples sent as part of Trial III along with the mean values from this Trial for SRM 1649a are summarized in Table 8. The z-scores and p-scores by laboratory are summarized in Table 9 along with the number of compounds reported by each laboratory. Since the laboratories, in general, ran the samples in one batch the p-scores only indicate a intra-batch precision, which is generally better than an inter-batch precision. The percentage of z-scores and p-scores in ranges of values are summarized below:

	absolute value of z scores (25%)				absolute value of z scores (s)				absolute value of p scores (15%)			
	0 to 1	1 to 2	2 to 3	>3	0 to 1	1 to 2	2 to 3	>3	0 to 1	1 to 2	2 to 3	>3
SRM 1648	67.9%	17.1%	7.2%	7.8%	64.6%	27.6%	1.2%	6.6%	84.0%	7.4%	4.3%	4.3%
Baltimore-2 PM	52.4%	26.2%	10.5%	10.9%	70.6%	23.6%	1.3%	4.5%	76.4%	11.6%	4.2%	7.8%
RM 8785	36.5%	25.9%	16.4%	21.2%	68.0%	22.5%	1.8%	7.6%	26.6%	34.7%	15.3%	23.4%
SRM 1649a									82.1%	11.7%	3.6%	2.6%

In general, the agreement among the laboratories was the best for SRM 1648. The concentrations of the majority of the analytes in SRM 1648 are similar to those in SRM 1649a while the concentrations of the analytes in Baltimore-2 PM tended to be lower than those in SRM 1649a. The data for the filter material, RM 8785, represented the most spread among the laboratories as expected. The filters contained between 0.3 mg and 3 mg of resuspended fine fraction from SRM 1649a. The data indicate that the laboratories were challenged by the limited sample size as the z-scores and p-scores were higher for this material. As seen in the above table, 21% of the data submitted for RM 8785 were >75% from the exercise assigned values [z-score(25%) >3], and 23% of the three data points submitted by individual laboratories varied by > 45% [p-score(15%) >3]. Since many laboratories are routinely analyzing PM on filters, the disparity of these data should be considered when comparing data across laboratories or even within one laboratory.

Intercomparison exercises provide an important mechanism for assessing the comparability, accuracy, and reproducibility of results from the participating laboratories. Exercise materials similar in matrix, form, and analyte concentration to typical samples routinely analyzed by the laboratories are most useful for demonstrating the level of comparability and for revealing potential problem areas. Minimizing the between-laboratory bias so that the analytical variability is significantly less than the sampling variability should be an achievable goal.

Problems and Potential Solutions for Improving Quantification of Target Analytes

PAHs: Eleven laboratories returned data for selected PAHs in SRM 1648 and Baltimore-2 PM while twelve laboratories returned data for selected PAHs in RM 8785. This is the largest data set received for any of the analyte groups. PAH analysis is fairly well-established with a number of commercial sources for neat chemicals of stated purity as well as a number of commercial sources of reliable calibration solutions. In addition, SRMs exist for PAHs in solution as well as natural matrices such as air particulate matter and sediment. Some problems were noted for individual analytes, however. There was a wide variation in the data received for naphthalene, ranging from 300 ng/g to 15700 ng/g in SRM 1648 and from 300 ng/g to 66000 ng/g in Baltimore-2PM. Naphthalene is a volatile compound, so it is important to have an internal standard/surrogate added to the samples that will mimic the behavior of naphthalene during the sample preparation steps, preferably carbon-13 or deuterium labeled naphthalene. The majority of the laboratories reporting data for chrysene neglected to note a coelution with triphenylene. These isomers coelute on most gas chromatographic phases, but they can be partially separated using a 60 m nonpolar column (5%, mole fraction, phenyl methylpolysiloxane phase) and almost baseline separated using a 60 m proprietary phase (DB-XLB), both with a slow temperature program. [5] A number of laboratories also misidentified the benzofluoranthene isomers. There are three isomers that elute close to one another, the *b*, *j*, and *k* isomers. Typically, benzo[*b*]fluoranthene and benzo[*j*]fluoranthene coelute on the nonpolar columns, including the DB-XLB mentioned above. A moderately polar 50% phenyl methylpolysilxoane phase, however, will separate the isomers, and depending on the operating conditions may change the elution order for the benzo[*j*] and benzo[*k*]fluoranthenes [5]. A

combined concentration for dibenz[*a,h*]anthracene and dibenz[*a,c*]anthracene was also commonly reported by the participants as only dibenz[*a,h*]anthracene. These two isomers coelute on the non-polar phases but can be separated on the moderately polar phases. There were only very limited data (six sets or fewer) received for some of the potentially more interesting PAHs, including the methylphenanthrenes, retene, coronene, and dibenzo[*a,e*]pyrene. These compounds were in the SRMs provided (SRM 2260a and 1491a) to the laboratories requesting them so it is unclear why more laboratories did not report values.

Nitrated-PAHs: Only two laboratories returned data for the nitrated-PAHs in SRM 1648 and Baltimore-2 PM, and three laboratories returned data for the nitrated-PAHs in RM 8785. The agreement among the two laboratories was within 20% for the nitrated-PAHs in SRM 1648 and Baltimore-2 PM; however, the agreement among the three laboratories was worse (70% relative standard deviation) for 1-nitropyrene and 2-nitrofluoranthene in RM 8785. SRMs 2264 and 2265 contain all of the compounds of interest in these studies along with additional nitrated-PAHs.

PAH-Quinones: Two laboratories returned data for the PAH-quinones in SRM 1648 and Baltimore-2 PM while only one laboratory returned data for the PAH-quninones in RM 8785. The agreement was not good among the data from the two laboratories for the PAH-quinones in SRM 1648 or in Baltimore-2 PM (>20% relative standard deviation). Other laboratories in the working group have expressed interest in quantifying PAH-quinones but did not do so in this trial.

Alkanes and alkenes: Eight laboratories returned data for selected alkanes in SRM 1648 and Baltimore-2 PM, and seven laboratories returned data for selected alkanes in RM 8785. No data sets were returned for the alkenes. For all of the samples, there was a large spread in the data reported for the alkanes with relative standard deviations >25% except for C-21 in RM 8785 (relative standard deviation of 2.3%). This spread in the alkane data is probably due to the non-specificity of the mass spectral ion/ions that are used to monitor alkanes. The alkanes tend to fragment in the mass spectrometer resulting in low relative molecular mass (<100) fragments that are commonly used to identify and quantify the alkanes. Other substituted alkanes, however, may fragment to a similar pattern resulting in misidentification. In addition, alkanes are commonly found in laboratory blanks so overestimation of the alkane concentrations is a possibility if blanks are not monitored. SRM 1494 was available at the start of this study. Many of the laboratories receiving SRM 1494, however, did not return data for the trial.

Hopanes, cholestanes, and sterols: Four laboratories (not the same four for all samples) reported data for this class of compounds in Trial III. The agreement among the laboratories for four of the hopanes and steranes in SRM 1648 (Table 1) and one hopane in Baltimore-2PM (Table 2) is quite good (<10% relative standard deviation). The relative standard deviations for the remainder of the hopanes, cholestanes, and sterols is >20%. As for the alkanes, there is one mass spectral fragment ion that is typically used to quantify the hopanes (191) and two that are typically used to quantify the steranes (217 and 218). Due to the lack of available standards, the correct identification of the hopanes and steranes is an issue. Candidate SRM 2266 contains the

10 hopanes and steranes targeted in Trial III. Only a limited number of laboratories, however, requested this solution.

Carbonyls and acids: Three laboratories returned data for hexadecanoic acid in SRM 1648 and Baltimore-2 PM. The relative standard deviation of the consensus value for both samples was > 50 %. Two laboratories returned data for hexadecanoic acid in RM 8785 with values differing by a factor of 2.7. One of those laboratories reported data for pimaric acid and isopimaric acid in RM 8785 as well. Due to the polarity of these compounds, there are additional analytical challenges, both in extraction and isolation from the matrix. Many of these compounds need to be derivatized prior to gas chromatographic analysis. A subgroup of the PM2.5 Organic Speciation Working Group has identified a list of acids and deuterated acids that will be used to prepare two future SRM solutions for use in quantifying acids in various matrices.

Phenols and sugars: Only laboratory 11 reported data for selected phenols in the three samples. The only sugar on the target analyte list currently is levoglucosan. Three laboratories reported values for levoglucosan in SRM 1648 and Baltimore-2 PM with relative standard deviations of 70% and 80%, respectively. Two laboratories reported values of levoglucosan in RM 8785 with a factor of 1.8 difference between the two values. These polar compounds present challenges similar to those of the carbonyls and acids. Solutions of deuterated and carbon-13 labeled levoglucosan (Candidate SRM 2267 and 2268, respectively) were sent to additional laboratories who did not return data for levoglucosan in this trial.

Conclusions and Recommendations

For the PAHs, the agreement among the laboratories submitting data for trial III was generally good except for those compounds with known coelutions. Neat chemicals of known purity and well-characterized solutions are available for the PAHs. For the nitrated-PAHs, only a limited number of laboratories experienced in this area submitted data so the agreement among the data was also good except for two nitrated-PAHs in RM 8785. The data received for the remaining classes of compounds showed a wide variation. This variation is probably due to a number of factors, including modifications needed in the extraction and isolation methods used for more polar compounds, mass spectral fragmentation, and chromatographic interferences. An effort is currently underway at NIST to produce additional calibration solution SRMs for a number of the compounds and labeled analogues. Several of these materials were made available to the participants in Trial III, but a number of the laboratories requesting the solutions did not return data thus making it difficult to assess whether the solutions helped or not.

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Disclaimer

Certain commercial equipment, instruments, or materials are identified in this report to specify adequately the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are the best available for the purpose.

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Table 1. SRM 1648		Laboratory means of three replicates and exercise assigned values																			
ng/g (reported as if three figures were significant)																					
PAHs																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
naphthalene	1324	NA	753	1123	NA	NA	NA	NA	NA	**15716**	1573	659	NA	NA	1711	831	NA	326	1038	479	46.1
fluorene	270	299	225	257	NA	NA	NA	NA	151	242	260	194	NA	NA	**594**	DL	NA	285	242	46	19.1
phenanthrene	5616	5646	5140	5043	NA	NA	NA	NA	3786	3977	3490	4315	NA	NA	4893	2202	NA	3470	4325	1061	24.5
anthracene	458	460	416	500	NA	NA	NA	NA	528	346	343	678	NA	NA	953	**535**	NA	440	463	102	21.9
1-methylphenanthrene	453	465	465	NA	NA	NA	NA	NA	NA	NA	420	319	NA	NA	835	DL	NA	NA	424	62	14.6
2-methylphenanthrene	968	954	895	NA	NA	NA	NA	NA	NA	NA	750	373	NA	NA	1074	DL	NA	NA	928	119	12.8
3-methylphenanthrene	741	714	718	NA	NA	NA	NA	NA	NA	NA	613	DL	NA	NA	826	DL	NA	NA	722	76	10.5
9-methylphenanthrene	440	419	415	NA	NA	NA	NA	NA	NA	NA	393	DL	NA	NA	582	DL	NA	NA	450	76	16.9
retene	757	738	NA	NA	NA	NA	NA	NA	NA	446	183	431	NA	NA	<80	DL	NA	NA	511	240	46.9
4H-cyclopenta[*def*]phenanthrene	306.0	318	300	NA	NA	NA	NA	NA	**600**	NA	213	NA	NA	NA	NA	DL	NA	NA	284	48	16.9
fluoranthene	8757	8975	8811	8763	NA	NA	NA	NA	8829	7037	7733	8021	NA	NA	7181	**3029**	NA	6798	8091	849	10.5
pyrene	6901	6871	6356	6200	NA	NA	NA	NA	6659	5778	5263	6816	NA	NA	6561	**2390**	NA	5170	6258	647	10.3
benzo[*ghi*]fluoranthene	1245	1216	1109	NA	NA	NA	NA	NA	**2460**	971	NA	NA	NA	NA	**2768**	DL	NA	NA	1135	124	10.9
cyclopenta[*cd*]pyrene	236	220	199	NA	NA	NA	NA	NA	**931**	NA	163	NA	NA	NA	**473**	278	NA	NA	219	43	19.4
benz[*a*]anthracene	2938	2951	2720	3037	NA	NA	NA	NA	**4835**	2784	3803	2410	NA	NA	**4729**	1225	NA	2015	2654	722	27.2
chrysene	NA	6146	NA	5773	NA	NA	NA	NA	NA	5242	NA	5843	NA	NA	3491	**1128**	NA	4478	5162	1007	19.5
triphenylene	NA	2179	NA	NA	NA	NA	NA	NA	NA	1958	NA	NA	NA	NA	2720	1554	NA	NA	2103	486	23.1
benzo[*b*]fluoranthene	9139	9292	9574	10287	NA	NA	NA	NA	NA	11963	9033	8599	NA	NA	NA	**3817**	6481	6441	8979	1729	19.3
benzo[*j*]fluoranthene	3346	3318	3549	NA	NA	NA	NA	NA	NA	NA	2733	NA	NA	NA	NA	NA	NA	NA	3237	351	10.8
benzo[*k*]fluoranthene	3242	3222	3261	3793	NA	NA	NA	NA	NA	NA	**2800**	3099	NA	NA	NA	NA	**5778**	2753	3228	336	10.4
benzo[*e*]pyrene	5163	5463	5587	NA	NA	NA	NA	NA	5609	5008	5257	7147	NA	NA	4542	2309	3041	NA	4913	1368	27.8
benzo[*a*]pyrene	2731	2724	2572	2733	NA	NA	NA	NA	3070	2483	1983	3046	NA	NA	2377	**589**	NA	2293	2601	335	12.9
perylene	765	732	690	NA	NA	NA	NA	NA	777	624	533	NA	NA	NA	655	DL	NA	NA	682	86	12.6
indeno[1,2,3-*cd*]pyrene	4243	4234	3928	4600	NA	NA	NA	NA	5702	4474	NA	3051	NA	NA	4362	DL	NA	3093	4187	801	19.1
benzo[*ghi*]perylene	5371	5265	4880	5090	NA	NA	NA	NA	5119	4513	5937	4234	NA	NA	5928	**2099**	NA	4723	5106	555	10.9
dibenz[*a,h*]anthracene	557	559	NA	453	NA	NA	NA	NA	NA	**651**	NA	316	NA	NA	NA	DL	NA	449	467	100	21.4
dibenz[*a,c*]anthracene	438	449	535	NA	NA	NA	NA	NA	NA	NA	377	NA	NA	NA	NA	DL	NA	NA	450	65	14.5
benzo[*b*]chrysene	435	424	404	NA	NA	NA	NA	NA	386	28.7	283	NA	NA	NA	**508**	DL	NA	NA	386	61	15.7
coronene	2668	2703	2229	2663	NA	NA	NA	NA	**5862**	NA	3127	NA	NA	NA	2399	DL	NA	NA	2632	306	11.6
dibenzo[*a,e*]pyrene	650	605	760	NA	NA	NA	NA	NA	**2530**	NA	543	NA	NA	NA	**770**	DL	NA	NA	640	92	14.3
Nitro-PAH ANALYSES																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
9-nitroanthracene	167	NA	NA	NA	NA	NA	NA	NA	NA	169	NA	NA	NA	NA	NA	NA	NA	NA	168	1	0.8
1-nitropyrene	92.0	NA	NA	NA	NA	NA	NA	NA	NA	68.6	NA	NA	NA	NA	NA	NA	NA	NA	80	17	20.6
2-nitrofluoranthene	252	NA	NA	NA	NA	NA	NA	NA	NA	343	NA	NA	NA	NA	NA	NA	NA	NA	297	64	21.5
3-nitrofluoranthene	6.82	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
7-nitrobenz[*a*]anthracene	78.4	NA	NA	NA	NA	NA	NA	NA	NA	89	NA	NA	NA	NA	NA	NA	NA	NA	84	7	8.9
6-nitrochrysene	<10	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
6-nitrobenzo[*a*]pyrene	<20	NA	NA	NA	NA	NA	NA	NA	NA	11.7	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 1. Continued																					
PAH-Quinone ANALYSES																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
1,2-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
1,4-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9-fluoreneone	NA	NA	NA	NA	NA	NA	NA	827	NA	NA	NA	NA	NA	NA	1168	NA	NA	NA	998	241	24.2
acenaphthenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	670	NA	NA	NA	No assigned value		
perinaphthenone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2322	NA	NA	NA	No assigned value		
anthraquinone (9,10-AQ)	NA	NA	NA	NA	NA	NA	NA	3115	NA	NA	NA	NA	NA	NA	4100	NA	NA	NA	3607	697	19.3
benzanthrone	NA	NA	NA	NA	NA	NA	NA	252	NA	NA	NA	NA	NA	NA	1795	NA	NA	NA	1024	1091	106.6
benz[*a*]anthracene-7,12-dione	NA	NA	NA	NA	NA	NA	NA	3987	NA	NA	NA	NA	NA	NA	2255	NA	NA	NA	3121	1225	39.2
1,4-chrysenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<80	NA	NA	NA	No assigned value		
Alkanes and Alkenes																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
n-C20	2723	NA	1053	NA	NA	NA	NA	1792	NA	NA	NA	**19546**	2103	NA	2350	4825	NA	NA	2474	1283	51.8
n-C21	NA	NA	NA	NA	NA	NA	NA	1949	NA	NA	NA	NA	3600	NA	6042	2031	NA	NA	3406	1915	56.2
n-C22	5313	NA	4761	NA	NA	NA	NA	4146	NA	NA	NA	5240	6063	NA	9687	13079	NA	NA	6898	3268	47.4
n-C23	8707	NA	NA	NA	NA	NA	NA	6709	NA	NA	NA	NA	11200	NA	27177	6986	NA	NA	8400	2065	24.6
n-C24	18346	NA	26991	NA	NA	NA	NA	18342	NA	NA	NA	10022	29333	NA	**51609**	15922	12377	NA	18762	7130	38.0
n-C25	47779	NA	NA	NA	NA	NA	NA	50291	NA	NA	NA	NA	74667	NA	100071	27119	NA	NA	59986	28043	46.7
n-C26	41254	NA	69906	NA	NA	NA	NA	51291	NA	NA	NA	28696	72753	NA	66897	37548	31539	NA	49986	17838	35.7
n-C27	43677	NA	NA	NA	NA	NA	NA	43347	NA	NA	NA	NA	63667	NA	61246	19722	NA	NA	46332	17656	38.1
n-C28	20733	NA	33945	NA	NA	NA	NA	26386	NA	NA	NA	15242	37800	NA	29202	24590	10199	NA	24762	9224	37.3
n-C29	48244	NA	NA	NA	NA	NA	NA	40568	NA	NA	NA	NA	59667	NA	53070	26155	NA	NA	45541	12885	28.3
n-C30	13973	NA	18732	NA	NA	NA	NA	16649	NA	NA	NA	8525	21133	NA	21103	7323	5378	NA	14102	6320	44.8
n-C31	36863	NA	NA	NA	NA	NA	NA	36308	NA	NA	NA	NA	43867	NA	44972	7340	NA	NA	33870	15345	45.3
n-C32	10620	NA	11093	NA	NA	NA	NA	16050	NA	NA	NA	7102	10900	NA	11422	6965	3199	NA	9669	3855	39.9
n-C40	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1190	11459	NA	NA	No assigned value		
n-C44	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
squalene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
1-octadecene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 1. Continued																					
Hopanes, Cholestanes, Sterols																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1220	NA	NA	NA	NA	NA	No assigned value		
abb 20R 24R-Ethylcholestane (Chiron#0662,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1663	NA	NA	NA	NA	NA	No assigned value		
abb 20R 24S-Methylcholestane (Chiron#0643,28)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	810	NA	NA	NA	NA	NA	No assigned value		
abb 20R Cholestane (Chiron#0602,27)	1342	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1483	NA	NA	NA	NA	NA	1413	100	7.1
aaa 20R-Cholestane (Chiron#0622,27)	852	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	807	NA	NA	NA	NA	NA	830	32	3.9
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	1710	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1630	NA	NA	DL	1736	NA	1892	55	3.3
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	6567	NA	NA	DL	NA	NA	No assigned value		
17a(H),21b(H)-Hopane (Chiron#0132,30)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	9733	NA	NA	28510	12866	NA	17037	10059	59.0
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	5133	NA	NA	DL	2902	NA	4018	1578	39.3
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	3900	NA	NA	DL	3406	NA	3853	349	9.8
pristane	<1000	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<1900	NA	NA	DL	NA	NA	No assigned value		
phytane	478	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<1900	NA	775	DL	NA	NA	628	210	33.5
cholesterol	NA	NA	NA	NA	NA	NA	NA	2803	NA	NA	NA	NA	NA	NA	861	8773	NA	NA	4146	4123	99.5
stigmasterol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	No assigned value		
Carbonyls and Acids																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	8	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
G-nonanoic lactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
G-decanolactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9-anthraldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
syringaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
pimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	No assigned value		
isopimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1128	NA	NA	NA	No assigned value		
pinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
pinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	758	NA	NA	No assigned value		
hexadecanoic acid	NA	NA	NA	NA	NA	NA	NA	242344	NA	NA	NA	NA	NA	NA	313939	93943.8	NA	NA	218742	112210	51.8
norpinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
norpinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
nopinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
pinonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
caronaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 1. Continued																					
Phenols																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
syringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	155	NA	NA	NA	No assigned value		
4-ethylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
isoeugenol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	183	NA	NA	NA	No assigned value		
propionylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
butyrylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
guaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	No assigned value		
4-methylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	No assigned value		
4-ethylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	No assigned value		
Sugars																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
levoglucosan	NA	NA	NA	NA	NA	NA	NA	42347	NA	NA	NA	NA	NA	NA	86541	176953	NA	NA	101947	68612	67.3

Table 2. Baltimore-2 PM		Laboratory means of three replicates and exercise assigned values																			
ng/g (reported as if three figures were significant)																					
PAHs																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
naphthalene	957	NA	398	1265	NA	NA	NA	NA	NA	66090	4540	357	NA	NA	5627	2260	NA	831	2029	1997	98.4
fluorene	173	118	97.8	168	NA	NA	NA	NA	85.5	403	207	663	NA	NA	1646	DL	NA	127	227	189	83.5
phenanthrene	1115	1037	896	732	NA	NA	NA	NA	407	1034	1423	824	NA	NA	1143	522	NA	888	911	289	31.7
anthracene	82.2	85.1	94.1	68.0	NA	NA	NA	NA	<158	131	233	168	NA	NA	<350	DL	NA	82.4	118	57	48.3
1-methylphenanthrene	118	121	138	NA	NA	NA	NA	NA	NA	NA	287	118	NA	NA	438	DL	NA	NA	158	74	47.4
2-methylphenanthrene	274	274	268	NA	NA	NA	NA	NA	NA	NA	810	159	NA	NA	381	DL	NA	NA	397	234	58.8
3-methylphenanthrene	181	180	192	NA	NA	NA	NA	NA	NA	NA	300	DL	NA	NA	<350	DL	NA	NA	208	82	30.0
9-methylphenanthrene	111	112	125	NA	NA	NA	NA	NA	NA	NA	310	DL	NA	NA	<350	DL	NA	NA	164	97	59.1
retene	125	119	NA	NA	NA	NA	NA	NA	NA	85.1	157	480	NA	NA	<350	DL	NA	NA	189	166	87.8
4H-cyclopenta[*def*]phenanthrene	50.8	43.4	47.1	NA	NA	NA	NA	NA	261	NA	287	NA	NA	NA	NA	DL	NA	NA	107	120	112.0
fluoranthene	1728	1839	1332	1058	NA	NA	NA	NA	866	1148	353	1302	NA	NA	1299	444	NA	1343	1137	437	38.4
pyrene	1343	1340	1086	1023	NA	NA	NA	NA	895	1028	1743	1138	NA	NA	1410	627	NA	1149	1182	294	25.3
benzo[*ghi*]fluoranthene	234	232	286	NA	NA	NA	NA	NA	142	150	NA	NA	NA	NA	805	DL	NA	NA	225	56	25.0
cyclopenta[*cd*]pyrene	134	123	92	NA	NA	NA	NA	NA	115	NA	DL	NA	NA	NA	<350	DL	NA	NA	118	18	15.4
benz[*a*]anthracene	323	315	293	278	NA	NA	NA	NA	<186	298	527	252	NA	NA	429	DL	NA	295	294	23	8.0
chrysene	NA	1016	NA	607	NA	NA	NA	NA	NA	735	NA	841	NA	NA	1152	DL	NA	811	860	196	22.8
triphenylene	NA	381	NA	NA	NA	NA	NA	NA	NA	292	NA	NA	NA	NA	593	DL	NA	NA	415	158	38.0
benzo[*b*]fluoranthene	1332	1306	1254	983	NA	NA	NA	NA	NA	1308	2227	1078	NA	NA	NA	DL	NA	1181	1334	381	28.6
benzo[*j*]fluoranthene	515	512	528	NA	NA	NA	NA	NA	NA	NA	1463	NA	NA	NA	NA	DL	NA	NA	755	473	82.8
benzo[*k*]fluoranthene	424	475	464	338	NA	NA	NA	NA	NA	NA	1260	417	NA	NA	NA	DL	NA	426	424	48	11.4
benzo[*e*]pyrene	956	954	838	NA	NA	NA	NA	NA	437	881	913	1060	NA	NA	1206	DL	NA	NA	881	238	26.8
benzo[*a*]pyrene	456	475	442	332	NA	NA	NA	NA	263	319	277	820	NA	NA	610	DL	NA	416	421	126	30.0
perylene	124	113	122	NA	NA	NA	NA	NA	<187	<167	DL	NA	NA	NA	431	DL	NA	NA	198	158	78.8
indeno[1,2,3-*cd*]pyrene	733	784	685	532	NA	NA	NA	NA	853	660	NA	643	NA	NA	913	DL	NA	660	718	115	16.1
benzo[*ghi*]perylene	1341	1221	1084	868	NA	NA	NA	NA	757	799	2180	859	NA	NA	1586	DL	NA	1057	1175	440	37.4
dibenz[*a,h*]anthracene	78.7	84.8	NA	46	NA	NA	NA	NA	NA	<100	NA	64	NA	NA	NA	DL	NA	65.2	87.7	15.2	22.5
dibenz[*a,c*]anthracene	104	97.8	92.7	NA	NA	NA	NA	NA	NA	NA	DL	NA	NA	NA	NA	DL	NA	NA	98.2	5.8	5.9
benzo[*b*]chrysene	52.6	57.6	59.7	NA	NA	NA	NA	NA	<173	<200	DL	NA	NA	NA	490	DL	NA	NA	56.6	3.8	6.4
coronene	600	559	490	385	NA	NA	NA	NA	539	NA	750	NA	NA	NA	788	DL	NA	NA	587	142	24.1
dibenzo[*a,e*]pyrene	183	<200	176	NA	NA	NA	NA	NA	<96	NA	DL	NA	NA	NA	<350	DL	NA	NA	170	9	5.6
Nitro-PAH ANALYSES																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
9-nitroanthracene	80.4	NA	NA	NA	NA	NA	NA	NA	NA	83.5	NA	NA	NA	NA	NA	NA	NA	NA	81.9	2.2	2.7
1-nitropyrene	36.1	NA	NA	NA	NA	NA	NA	NA	NA	28.7	NA	NA	NA	NA	NA	NA	NA	NA	32.4	5.2	18.2
2-nitrofluoranthene	313	NA	NA	NA	NA	NA	NA	NA	NA	319	NA	NA	NA	NA	NA	NA	NA	NA	318	5	1.5
3-nitrofluoranthene	<10	NA	NA	NA	NA	NA	NA	NA	NA	<4	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
7-nitrobenz[*a*]anthracene	<10	NA	NA	NA	NA	NA	NA	NA	NA	<10	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
6-nitrochrysene	<10	NA	NA	NA	NA	NA	NA	NA	NA	<6	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
6-nitrobenzo[*a*]pyrene	<10	NA	NA	NA	NA	NA	NA	NA	NA	<6	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		

Table 2. Continued																					
PAH-Quinone ANALYSES																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
1,2-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
1,4-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9-fluorenenone	NA	NA	NA	NA	NA	NA	NA	295	NA	NA	NA	NA	NA	NA	430.8	NA	NA	NA	363	96	26.4
acenaphthenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	516.2	NA	NA	NA	No assigned value		
perinaphthenone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<350	NA	NA	NA	No assigned value		
anthraquinone (9,10-AQ)	NA	NA	NA	NA	NA	NA	NA	376	NA	NA	NA	NA	NA	NA	940.0	NA	NA	NA	658	399	60.6
benzanthrone	NA	NA	NA	NA	NA	NA	NA	339	NA	NA	NA	NA	NA	NA	1026.0	NA	NA	NA	682	486	71.2
benz[*a*]anthracene-7,12-dione	NA	NA	NA	NA	NA	NA	NA	774	NA	NA	NA	NA	NA	NA	1257.0	NA	NA	NA	1015	342	33.6
1,4-chrysenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	414.6	NA	NA	NA	No assigned value		
Alkanes and Alkenes																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
n-C20	2933	NA	3980	NA	NA	NA	NA	1060	NA	NA	NA	32807	<1900	NA	5189	1961	NA	NA	3025	1628	53.8
n-C21	NA	NA	NA	NA	NA	NA	NA	513	NA	NA	NA	NA	2190	NA	8820	2428	NA	NA	3488	3655	104.8
n-C22	1888	NA	2612	NA	NA	NA	NA	1542	NA	NA	NA	1556	2633	NA	15794	3664	NA	NA	2316	821	35.4
n-C23	5739	NA	NA	NA	NA	NA	NA	2376	NA	NA	NA	NA	6800	NA	64816	6631	NA	NA	5387	2060	38.2
n-C24	3169	NA	4613	NA	NA	NA	NA	1391	NA	NA	NA	1597	6067	NA	51000	3875	4311	NA	3575	1672	46.8
n-C25	10751	NA	NA	NA	NA	NA	NA	4113	NA	NA	NA	NA	16333	NA	59841	9765	NA	NA	10240	5005	48.9
n-C26	5861	NA	7146	NA	NA	NA	NA	2728	NA	NA	NA	17339	10633	NA	15702	9429	6881	NA	9465	4967	52.5
n-C27	27344	NA	NA	NA	NA	NA	NA	10407	NA	NA	NA	NA	30667	NA	32350	16081	NA	NA	23370	9629	41.2
n-C28	15676	NA	9696	NA	NA	NA	NA	3666	NA	NA	NA	16617	13667	NA	12805	13485	9829	NA	11930	4139	34.7
n-C29	31073	NA	NA	NA	NA	NA	NA	21140	NA	NA	NA	NA	54667	NA	57332	30986	NA	NA	39039	16028	41.1
n-C30	10252	NA	9134	NA	NA	NA	NA	2902	NA	NA	NA	13204	10700	NA	10622	4988	11694	NA	9187	3486	37.9
n-C31	29933	NA	NA	NA	NA	NA	NA	17553	NA	NA	NA	NA	45000	NA	52216	15332	NA	NA	32007	16344	51.1
n-C32	8199	NA	21577	NA	NA	NA	NA	2045	NA	NA	NA	10026	6833	NA	7738	8209	12376	NA	9625	5650	58.7
n-C40	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1405	4254	NA	NA	No assigned value		
n-C44	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
squalene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
1-octadecene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 2. Continued																					
Hopanes, Cholestanes, Sterols																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	123	217	NA	NA	NA	NA	No assigned value		
abb 20R 24R-Ethylcholestane (Chiron#0662,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	153	477	NA	NA	NA	NA	No assigned value		
abb 20R 24S-Methylcholestane (Chiron#0643,28)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<80	517	NA	NA	NA	NA	No assigned value		
abb 20R Cholestane (Chiron#0602,27)	<500	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	157	600	NA	NA	NA	NA	No assigned value		
aaa 20R-Cholestane (Chiron#0622,27)	132	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<80	367	NA	NA	NA	NA	249	168	66.7
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	170	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	187	243	NA	**16735**	NA	NA	193	43	22.4
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	787	707	NA	DL	NA	NA	747	57	7.8
17a(H),21b(H)-Hopane (Chiron#0132,30)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	767	950	NA	51837	NA	NA	No assigned value		
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	700	527	NA	DL	NA	NA	No assigned value		
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	583	580	NA	DL	NA	NA	No assigned value		
pristane	<1000	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<1900	NA	NA	816	NA	NA	No assigned value		
phytane	<1000	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<1900	NA	1075	1429	NA	NA	1252	250	20.0
cholesterol	NA	NA	NA	NA	NA	NA	NA	5303	NA	NA	NA	NA	NA	NA	4593	38742	NA	NA	16213	19514	120.4
stigmasterol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	5817	NA	NA	NA	No assigned value		
Carbonyls and Acids																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	8	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
G-nonanoic lactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
G-decanolactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9-anthraldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
syringaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
pimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1061	NA	NA	NA	No assigned value		
isopimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1097	NA	NA	NA	No assigned value		
pinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
pinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	DL	NA	NA	No assigned value		
hexadecanoic acid	NA	NA	NA	NA	NA	NA	NA	96829	NA	NA	NA	NA	NA	NA	240585	100548	NA	NA	145987	81945	56.1
norpinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
norpinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
nopinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
pinonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
caronaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 2. Continued																					
Phenols																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
syringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<730	NA	NA	NA	No assigned value		
4-ethylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
isoeugenol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<730	NA	NA	NA	No assigned value		
propionylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
butyrylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
guaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<730	NA	NA	NA	No assigned value		
4-methylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<730	NA	NA	NA	No assigned value		
4-ethylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<730	NA	NA	NA	No assigned value		
Sugars																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
levoglucosan	NA	NA	NA	NA	NA	NA	NA	13489	NA	NA	NA	NA	NA	NA	121289	183751	NA	NA	106176	86131	81.1

Table 3. RM 8785 Air Particulate on Filter		Laboratory means of three replicates and exercise assigned values																			
ng/g (reported as if three figures were significant)																					
PAHs																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
naphthalene	1422	NA	5428	**47213**	1482	6665	NA	NA	NA	**1603575**	DL	2032	NA	NA	**240250**	12567	NA	770	4338	4263	98.3
fluorene	236	<2400	1050	5680	944	817	535	NA	NA	6750	DL	828	NA	NA	**46870**	DL	NA	NA	2355	3120	132.5
phenanthrene	4632	4485	6030	15453	2573	2713	16927	NA	NA	13325	DL	2418	NA	NA	16667	3663	NA	2319	7600	6061	79.7
anthracene	457	<1200	1282	1605	330	621	1945	NA	NA	2550	DL	871	NA	NA	**<15000**	DL	NA	543	1134	766	67.6
1-methylphenanthrene	462	527	1171	NA	NA	1185	NA	NA	NA	NA	DL	694	NA	NA	**<15000**	DL	NA	NA	808	349	43.2
2-methylphenanthrene	779	1130	2047	NA	NA	1015	NA	NA	NA	NA	DL	**756**	NA	NA	<15000	DL	NA	NA	1243	556	44.7
3-methylphenanthrene	554	875	1355	NA	NA	638	NA	NA	NA	NA	DL	DL	NA	NA	<15000	DL	NA	NA	856	360	42.1
9-methylphenanthrene	434	427	1037	NA	NA	703	NA	NA	NA	NA	DL	DL	NA	NA	<15000	DL	NA	NA	650	288	44.3
retene	339	DL	NA	NA	NA	NA	NA	NA	NA	<1400	DL	8362	NA	NA	<15000	DL	NA	NA	no assigned value		
4H-cyclopenta[*def*]phenanthrene	378.8	<1000	610	NA	NA	NA	NA	NA	NA	NA	DL	NA	NA	NA	NA	DL	NA	NA	no assigned value		
fluoranthene	5887	5498	5870	9985	4703	3850	7012	NA	NA	6125	DL	5327	NA	NA	12628	2197	NA	3609	6057	2829	46.7
pyrene	3829	3422	5033	8295	3375	3093	7179	NA	NA	6050	DL	4722	NA	NA	13460	1938	NA	2651	5254	3200	60.9
benzo[*ghi*]fluoranthene	1280	1287	**3526**	NA	NA	NA	NA	NA	NA	1200	NA	NA	NA	NA	**13307**	DL	NA	NA	1256	48	3.8
cyclopenta[*cd*]pyrene	<500	860	944	NA	NA	NA	NA	NA	NA	NA	DL	NA	NA	NA	**9390**	DL	NA	NA	902	59	6.6
benz[*a*]anthracene	2123	1984	2217	3620	1278	1263	1937	NA	NA	2725	DL	2480	NA	NA	**16518**	DL	NA	884	2051	798	38.9
chrysene	NA	3926	NA	5073	3400	2848	**9364**	NA	NA	3850	NA	5789	NA	NA	**15907**	DL	NA	2232	3874	1230	31.8
triphenylene	NA	2061	NA	NA	NA	NA	NA	NA	NA	2175	NA	NA	NA	NA	**12515**	DL	NA	NA	2118	81	3.8
benzo[*b*]fluoranthene	8155	9957	8421	NA	7730	7050	6297	NA	NA	10975	DL	11997	NA	NA	NA	DL	NA	5232	8424	2202	26.1
benzo[*j*]fluoranthene	2385	2688	2860	NA	NA	1910	NA	NA	NA	NA	DL	NA	NA	NA	NA	DL	NA	NA	2461	416	16.9
benzo[*k*]fluoranthene	2197	2441	2451	3713	2063	**4578**	1761	NA	NA	NA	DL	3449	NA	NA	NA	DL	NA	1689	2470	742	30.0
benzo[*e*]pyrene	4013	5013	4336	NA	NA	NA	4371	NA	NA	4525	DL	**39970**	NA	NA	**18668**	DL	NA	NA	4452	365	8.2
benzo[*a*]pyrene	2413	2385	2353	3413	2350	1285	2567	NA	NA	<9100	DL	**6381**	NA	NA	**18014**	DL	NA	1311	2395	619	25.9
perylene	391	<1000	1463	NA	NA	NA	392	NA	NA	<7600	DL	NA	NA	NA	**14926**	DL	NA	NA	748	619	82.7
indeno[1,2,3-*cd*]pyrene	4159	4350	4364	6743	4593	3838	4361	NA	NA	6250	NA	6161	NA	NA	**21364**	DL	NA	2549	4737	1279	27.0
benzo[*ghi*]perylene	6892	7359	6655	10870	7208	4643	6608	NA	NA	6850	DL	8339	NA	NA	**29886**	DL	NA	4267	6969	1834	26.3
dibenz[*a,h*]anthracene	<500	DL	NA	<900	407	**805**	323	NA	NA	<4600	NA	1940	NA	NA	NA	DL	NA	283	738	803	108.7
dibenz[*a,c*]anthracene	<500	DL	<730	NA	NA	NA	NA	NA	NA	NA	DL	NA	NA	NA	NA	DL	NA	NA	no assigned value		
benzo[*b*]chrysene	<500	DL	885	NA	NA	NA	NA	NA	NA	<9100	DL	NA	NA	NA	13058	DL	NA	NA	no assigned value		
coronene	5233	7617	7126	13985	NA	NA	NA	NA	NA	NA	DL	NA	NA	NA	17832	DL	NA	NA	10358	5321	51.4
dibenzo[*a,e*]pyrene	<800	DL	ND	NA	NA	NA	NA	NA	NA	NA	DL	NA	NA	NA	8806	DL	NA	NA	no assigned value		
Nitro-PAH ANALYSES																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
9-nitroanthracene	<50	NA	NA	NA	NA	NA	NA	49	NA	NA	44	NA	NA	NA	NA	NA	NA	NA	47	4	8.0
1-nitropyrene	111	NA	NA	NA	NA	NA	NA	347	NA	NA	109	NA	NA	NA	NA	NA	NA	NA	189	137	72.3
2-nitrofluoranthene	394	NA	NA	NA	NA	NA	1234	NA	NA	522	NA	NA	NA	NA	NA	NA	NA	NA	717	453	63.2
3-nitrofluoranthene	<20	NA	NA	NA	NA	NA	510	NA	NA	<4.70	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
7-nitrobenz[*a*]anthracene	<50	NA	NA	NA	NA	NA	76	NA	NA	51	NA	NA	NA	NA	NA	NA	NA	NA	63	18	27.9
6-nitrochrysene	<20	NA	NA	NA	NA	NA	253	NA	NA	<5.92	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
6-nitrobenzo[*a*]pyrene	<20	NA	NA	NA	NA	NA	DL	NA	NA	<14.72	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 3. Continued																					
PAH-Quinone ANALYSES																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
1,2-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
1,4-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9-fluoreneone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	8806	NA	NA	NA	No assigned value		
acenaphthenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	27286	NA	NA	NA	No assigned value		
perinaphthenone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	14913	NA	NA	NA	No assigned value		
anthraquinone (9,10-AQ)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	10603	NA	NA	NA	No assigned value		
benzanthrone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	28058	NA	NA	NA	No assigned value		
benz[*a*]anthracene-7,12-dione	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	22676	NA	NA	NA	No assigned value		
1,4-chrysenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	12720	NA	NA	NA	No assigned value		
Alkanes and Alkenes																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
n-C20	NA	NA	<41000	NA	NA	NA	21849	NA	NA	NA	NA	33312	27528	NA	67918	97380	NA	NA	49598	32176	64.9
n-C21	NA	NA	NA	NA	NA	NA	19908	NA	NA	NA	NA	NA	19015	NA	215302	19451	NA	NA	19458	446	2.3
n-C22	NA	NA	<39000	NA	NA	NA	18281	NA	NA	NA	NA	49032	27978	NA	200197	223754	NA	NA	103849	99679	96.0
n-C23	NA	NA	NA	NA	NA	NA	14321	NA	NA	NA	NA	NA	36568	NA	367237	57107	NA	NA	35999	21399	59.4
n-C24	NA	NA	<31000	NA	NA	NA	19761	NA	NA	NA	NA	33395	77572	NA	179872	163108	30693	NA	84067	70739	84.1
n-C25	NA	NA	NA	NA	NA	NA	21051	NA	NA	NA	NA	NA	150447	NA	262860	98900	NA	NA	133314	101428	76.1
n-C26	NA	NA	<24000	NA	NA	NA	19069	NA	NA	NA	NA	36758	170837	NA	195804	266034	100886	NA	131565	96266	73.2
n-C27	NA	NA	NA	NA	NA	NA	18545	NA	NA	NA	NA	NA	198785	NA	189302	985305	NA	NA	347984	432878	124.4
n-C28	NA	NA	<17000	NA	NA	NA	12135	NA	NA	NA	NA	27820	123238	NA	137648	309752	95883	NA	79345	56505	71.2
n-C29	NA	NA	NA	NA	NA	NA	17715	NA	NA	NA	NA	NA	185962	NA	182294	142025	NA	NA	131999	78746	59.7
n-C30	NA	NA	<12000	NA	NA	NA	13217	NA	NA	NA	NA	30048	72231	NA	117527	79140	89696	NA	66977	38732	57.8
n-C31	NA	NA	NA	NA	NA	NA	10260	NA	NA	NA	NA	NA	95063	NA	157823	13811	NA	NA	69239	70863	102.3
n-C32	NA	NA	<9000	NA	NA	NA	5734	NA	NA	NA	NA	23301	31576	NA	86446	103014	75800	NA	54312	39255	72.3
n-C40	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	22572	198267	NA	NA	No assigned value		
n-C44	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
squalene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
1-octadecene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 3. Continued																						
Hopanes, Cholestanes, Sterols																						
Laboratory No.																			Exercise Assigned			
	1a	1b	1c	2	3a	3b	4	5	8	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD	
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	3394	1722	NA	NA	NA	NA	No assigned value			
abb 20R 24R-Ethylcholestane (Chiron#0662,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	4300	5442	NA	NA	NA	NA	No assigned value			
abb 20R 24S-Methylcholestane (Chiron#0643,28)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2531	8752	NA	NA	NA	NA	No assigned value			
abb 20R Cholestane (Chiron#0602,27)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	5511	15384	NA	NA	NA	NA	No assigned value			
aaa 20R-Cholestane (Chiron#0622,27)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2024	7812	NA	NA	NA	NA	No assigned value			
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	4302	6484	NA	DL	NA	NA	No assigned value			
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	21410	13174	NA	DL	NA	NA	No assigned value			
17a(H),21b(H)-Hopane (Chiron#0132,30)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	22188	29799	NA	49628	NA	NA	33871	14165	41.8	
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	12299	8258	NA	DL	NA	NA	No assigned value			
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	10854	7909	NA	DL	NA	NA	No assigned value			
pristane	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<62000	NA	NA	22007	NA	NA	No assigned value			
phytane	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	18352	NA	64146	70452	NA	NA	50983	28435	55.8	
cholesterol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	50384	199119	NA	NA	124752	105172	84.3	
stigmasterol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	76857	NA	NA	NA	No assigned value			
Carbonyls and Acids																						
Laboratory No.																			Exercise Assigned			
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD	
G-nonanoic lactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
G-decanolactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
9-anthraldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
syringaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
pimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<30000	NA	NA	NA	No assigned value			
isopimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	31056	NA	NA	NA	No assigned value			
pinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
pinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	10614	NA	NA	No assigned value			
hexadecanoic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	4487983	1223892	NA	NA	2855937	2308061	80.8	
norpinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
norpinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
nopinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
pinionaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
caronaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value			
Note: Bolded values were not used in the calculation of the exercise assigned values.																						

Table 3. Continued																					
Phenols																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
syringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<30000	NA	NA	NA	No assigned value		
4-ethylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
isoeugenol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<30000	NA	NA	NA	No assigned value		
propionylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
butyrylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	No assigned value		
guaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<30000	NA	NA	NA	No assigned value		
4-methylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<30000	NA	NA	NA	No assigned value		
4-ethylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<30000	NA	NA	NA	No assigned value		
Sugars																					
Laboratory No.																			Exercise Assigned		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	Assigned	s	%RSD
levoglucosan	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	267046	146455	NA	NA	206751	85270	41.2

Table 4. SRM 1649a (Trial III)		Laboratory means of three replicates and certificate values																			
ng/g (reported as if three figures were significant)																					
PAHs																					
Laboratory No.																			From 1649a Certif.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
naphthalene	1341	NA	829	962	683	407	NA	NA	NA	27984	2277	525	NA	NA	1019	2947	NA	357	no target		Target
fluorene	231	298	195	174	272	187	302	NA	151	266	213	194	NA	NA	468	DL	NA	183	230	50	Reference
phenanthrene	4180	4653	4339	3930	2683	3273	4805	NA	3550	3427	2940	3876	NA	NA	4093	5187	NA	3858	4140	370	Certified
anthracene	440	417	393	399	314	630	867	NA	473	347	313	574	NA	NA	728	1049	NA	655	432	82	Certified
1-methylphenanthrene	386	436	395	NA	NA	363	NA	NA	NA	NA	360	237	NA	NA	566	DL	NA	NA	370.0	40.0	Reference
2-methylphenanthrene	756	894	768	NA	NA	517	NA	NA	NA	NA	883	259	NA	NA	978	DL	NA	NA	730	120	Reference
3-methylphenanthrene	547	657	602	NA	NA	382	NA	NA	NA	NA	513	DL	NA	NA	898	DL	NA	NA	500	50	Reference
9-methylphenanthrene	402	392	347	NA	NA	331	NA	NA	NA	NA	340	DL	NA	NA	434	DL	NA	NA	no target		Target
retene	322	285	NA	NA	NA	NA	NA	NA	NA	100	87	253	NA	NA	<80	DL	NA	NA	no target		Target
4H-cyclopenta[*def*]phenanthrene	334	309	271	NA	NA	NA	NA	NA	506	NA	203	NA	NA	NA	NA	DL	NA	NA	320.0	60	Reference
fluoranthene	6619	6819	6625	6233	5493	6003	8575	NA	7412	5506	5440	6658	NA	NA	5577	8292	NA	8308	6450	180	Certified
pyrene	5315	5440	5093	5327	5583	4517	5562	NA	5774	4700	4160	5933	NA	NA	5131	5287	NA	4989	5290	260	Certified
benzo[*ghi*]fluoranthene	884	953	860	NA	NA	NA	NA	NA	1878	751	NA	NA	NA	NA	1951	899	NA	NA	880	20	Reference
cyclopenta[*cd*]pyrene	357	323	240	NA	NA	NA	NA	NA	792	NA	217	NA	NA	NA	382	792	NA	NA	no target		Target
benz[*a*]anthracene	2312	2304	2114	2183	2113	2233	2268	NA	4371	2254	2490	2152	NA	NA	4329	2681	NA	2025	2210	73	Certified
chrysene	NA	3270	NA	2927	3100	2453	8634	NA	NA	2853	NA	3354	NA	NA	3845	1948	NA	2955	3049	80	Certified
triphenylene	NA	1400	NA	NA	NA	NA	NA	NA	NA	1309	NA	NA	NA	NA	2255	2125	NA	NA	1357	54	Certified
benzo[*b*]fluoranthene	6564	5823	6277	6550	4907	5570	5719	NA	NA	7415	5147	5694	NA	NA	NA	6822	6475	4260	6450	640	Certified
benzo[*j*]fluoranthene	1493	1851	2047	NA	NA	1680	NA	NA	NA	NA	1063	NA	NA	NA	NA	NA	NA	NA	1500	400	Reference
benzo[*k*]fluoranthene	1919	1843	1992	1810	1687	4733	2477	NA	NA	NA	1117	1885	NA	NA	NA	NA	NA	1604	1913	31	Certified
benzo[*e*]pyrene	3156	3321	3456	NA	NA	NA	2913	NA	3601	3109	2993	4264	NA	NA	2695	3654	3821	NA	3090.0	190	Certified
benzo[*a*]pyrene	2453	2459	2370	2613	2413	2370	2695	NA	2771	2287	1870	2630	NA	NA	2195	2079	NA	2321	2509	87	Certified
perylene	666	677	634	NA	NA	NA	592	NA	636	584	670	NA	NA	NA	706	DL	NA	NA	646	75	Certified
indeno[1,2,3-*cd*]pyrene	3263	3011	2898	3330	3030	3293	2386	NA	4260	3138	NA	2643	NA	NA	2810	2970	NA	2250	3180	720	Certified
benzo[*ghi*]perylene	4032	4391	4062	4163	5457	3377	3458	NA	4352	3728	4633	3596	NA	NA	4490	4881	NA	3582	4010.0	910.00	Certified
dibenz[*a,h*]anthracene	303	330	NA	282	284	660	188	NA	NA	456	NA	260	NA	NA	NA	DL	NA	350	266.0	23.0	Certified
dibenz[*a,c*]anthracene	230	354	388	NA	NA	NA	NA	NA	NA	NA	210	NA	NA	NA	NA	DL	NA	NA	200	25	Certified
benzo[*b*]chrysene	321	374	386	NA	NA	NA	NA	NA	379	26	243	NA	NA	NA	461	DL	NA	NA	315	13	Certified
coronene	3635	3741	2698	3270	NA	NA	NA	NA	9053	NA	3730	NA	NA	NA	3696	3631	NA	NA	no target		Target
dibenzo[*a,e*]pyrene	703	624	664	NA	NA	NA	NA	NA	2029	NA	383	NA	NA	NA	211	DL	NA	NA	830	80	Reference
Nitro-PAH ANALYSES																					
Laboratory No.																			From 1649a Certif.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
9-nitroanthracene	34.7	NA	NA	NA	NA	NA	41.0	NA	NA	32	NA	NA	NA	NA	NA	NA	NA	NA	33.4	6.1	Target
1-nitropyrene	68.0	NA	NA	NA	NA	NA	65.4	NA	NA	62	NA	NA	NA	NA	NA	NA	NA	NA	70.9	4.3	Target
2-nitrofluoranthene	300	NA	NA	NA	NA	NA	317	NA	NA	313	NA	NA	NA	NA	NA	NA	NA	NA	313.0	38	Target
3-nitrofluoranthene	5.03	NA	NA	NA	NA	NA	5.13	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
7-nitrobenz[*a*]anthracene	25.3	NA	NA	NA	NA	NA	29.7	NA	NA	23	NA	NA	NA	NA	NA	NA	NA	NA	27.8	6.7	Target
6-nitrochrysene	<10	NA	NA	NA	NA	NA	6.84	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	4.01	0.52	Target
6-nitrobenzo[*a*]pyrene	<10	NA	NA	NA	NA	NA	28.0	NA	NA	6	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 4. Continued																					
PAH-Quinone ANALYSES																					
Laboratory No.																			From 1649a Certif.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
1,2-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
1,4-naphthoquinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
9-fluoreneone	NA	NA	NA	NA	NA	NA	NA	1096	NA	NA	NA	NA	NA	NA	1185	NA	NA	NA	no target		Target
acenaphthenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	437	NA	NA	NA	no target		Target
perinaphthenone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1484	NA	NA	NA	no target		Target
anthraquinone (9,10-AQ)	NA	NA	NA	NA	NA	NA	NA	2577	NA	NA	NA	NA	NA	NA	2996	NA	NA	NA	no target		Target
benzanthrone	NA	NA	NA	NA	NA	NA	NA	572	NA	NA	NA	NA	NA	NA	993	NA	NA	NA	no target		Target
benz[*a*]anthracene-7,12-dione	NA	NA	NA	NA	NA	NA	NA	3846	NA	NA	NA	NA	NA	NA	1819	NA	NA	NA	no target		Target
1,4-chrysenequinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	80.5	NA	NA	NA	no target		Target
Alkanes and Alkenes																					
Laboratory No.																			From 1649a Certif.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
n-C20	2645	NA	2645	NA	NA	NA	3204	1426	NA	NA	NA	18662	<1900	NA	1554	2243	NA	NA	no target		Target
n-C21	NA	NA	NA	NA	NA	NA	3565	1043	NA	NA	NA	NA	2480	NA	4458	3000	NA	NA	no target		Target
n-C22	5090	NA	5090	NA	NA	NA	4687	3410	NA	NA	NA	3384	4537	NA	7570	5705	NA	NA	no target		Target
n-C23	12953	NA	NA	NA	NA	NA	14058	10597	NA	NA	NA	NA	17067	NA	29211	17209	NA	NA	no target		Target
n-C24	22214	NA	22214	NA	NA	NA	26156	18696	NA	NA	NA	8228	31000	NA	43684	31135	12588	NA	no target		Target
n-C25	65313	NA	NA	NA	NA	NA	76594	56122	NA	NA	NA	NA	95000	NA	85209	92772	NA	NA	no target		Target
n-C26	45178	NA	45178	NA	NA	NA	65736	66357	NA	NA	NA	25911	97333	NA	87088	101114	30602	NA	no target		Target
n-C27	56248	NA	NA	NA	NA	NA	58882	62420	NA	NA	NA	NA	93333	NA	86441	74678	NA	NA	no target		Target
n-C28	23924	NA	23924	NA	NA	NA	31448	33882	NA	NA	NA	10687	52333	NA	43581	50860	11703	NA	no target		Target
n-C29	54403	NA	NA	NA	NA	NA	54254	47188	NA	NA	NA	NA	83667	NA	76778	84132	NA	NA	no target		Target
n-C30	14702	NA	14702	NA	NA	NA	19671	20521	NA	NA	NA	8488	27000	NA	26826	17063	7186	NA	no target		Target
n-C31	33675	NA	NA	NA	NA	NA	31252	31638	NA	NA	NA	NA	50667	NA	50021	33133	NA	NA	no target		Target
n-C32	10435	NA	10435	NA	NA	NA	6514	12738	NA	NA	NA	6769	14100	NA	13038	13685	NA	NA	no target		Target
n-C40	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1112	DL	NA	NA	no target		Target
n-C44	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
squalene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
1-octadecene	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 4. Continued																					
Hopanes, Cholestanes, Sterols																					
Laboratory No.																			From 1649a Certif.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1467	NA	NA	NA	NA	NA	no target		Target
abb 20R 24R-Ethylcholestane (Chiron#0662,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2267	NA	NA	NA	NA	NA	no target		Target
abb 20R 24S-Methylcholestane (Chiron#0643,28)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1237	NA	NA	NA	NA	NA	no target		Target
abb 20R Cholestane (Chiron#0602,27)	634	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2167	NA	NA	NA	NA	NA	no target		Target
aaa 20R-Cholestane (Chiron#0622,27)	1522	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1167	NA	NA	NA	NA	NA	no target		Target
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	2127	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	2000	NA	NA	9211	4170	NA	no target		Target
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	9100	NA	NA	DL	NA	NA	no target		Target
17a(H),21b(H)-Hopane (Chiron#0132,30)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	11333	NA	NA	47192	21901	NA	no target		Target
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	6633	NA	NA	DL	6044	NA	no target		Target
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	4900	NA	NA	DL	5481	NA	no target		Target
pristane	<1000	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<1900	NA	NA	DL	NA	NA	no target		Target
phytane	464	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<1900	NA	1495	DL	NA	NA	no target		Target
cholesterol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	1963	29836	NA	NA	no target		Target
stigmasterol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	no target		Target
Carbonyls and Acids																					
Laboratory No.																			From 1649a Certif.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
G-nonanoic lactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
G-decanolactone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
9-anthraldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
syringaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
pimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	no target		Target
isopimaric acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	583.1	NA	NA	NA	no target		Target
pinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
pinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
hexadecanoic acid	NA	NA	NA	NA	NA	NA	NA	399599	NA	NA	NA	NA	NA	NA	601072	NA	NA	NA	no target		Target
norpinic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
norpinonic acid	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
nopinone	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
pinionaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
caronaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
Note: Bolded values were not used in the calculation of the exercise assigned values.																					

Table 4. Continued																					
Phenols																					
Laboratory No.																			From 1649a Cert#.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
syringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	213	NA	NA	NA	no target		Target
4-ethylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
isoeugenol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	584	NA	NA	NA	no target		Target
propionylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
butyrylsyringol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	no target		Target
guaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	no target		Target
4-methylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	205	NA	NA	NA	no target		Target
4-ethylguaiacol	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	<150	NA	NA	NA	no target		Target
Sugars																					
Laboratory No.																			From 1649a Cert#.		
	1a	1b	1c	2	3a	3b	4	5	6	7	8	9	10a	10b	11	12	13	14	conc.	95%CL	type
levoglucosan	NA	NA	NA	NA	NA	NA	NA	14348	NA	NA	NA	NA	NA	NA	70907	53574	NA	NA	no target		Target

Table 5. Z-scores (25%) for data reported in Trial III

Laboratory No.	1a			1b			1c		
	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785
naphthalene	1.1	-2.1	-2.7				-1.1	-3.2	1.0
fluorene	0.4	-0.9	-3.6	0.9	-2.0		-0.3	-2.3	-2.2
phenanthrene	1.2	0.9	-1.6	1.2	0.6	-1.6	0.8	-0.1	-0.8
anthracene	0.0	-1.2	-2.4	0.0	-1.1		-0.4	-0.8	0.5
1-methylphenanthrene	0.3	-1.0	-1.7	0.4	-0.9	-1.4	0.4	-0.5	1.8
2-methylphenanthrene	0.2	-1.2	-1.5	0.1	-1.2	-0.4	-0.1	-1.3	2.6
3-methylphenanthrene	0.1	-0.9	-1.4	0.0	-0.5	0.1	0.0	-0.3	2.3
9-methylphenanthrene	-0.1	-1.3	-1.3	-0.3	-1.3	-1.4	-0.3	-1.0	2.4
retene	1.9	-1.4		1.8	-1.5				
4H-cyclopenta[*def*]phenanthrene	0.3	-2.1		0.5	-2.4		0.2	-2.2	
fluoranthene	0.3	2.1	-0.1	0.4	1.8	-0.4	0.4	0.7	-0.1
pyrene	0.4	0.6	-1.1	0.4	0.6	-1.4	0.1	-0.3	-0.2
benzo[*ghi*]fluoranthene	0.4	0.2	0.1	0.3	0.1	0.1	-0.1	1.1	7.2
cyclopenta[*cd*]pyrene	0.3	0.6		0.0	0.2	-0.2	-0.4	-0.8	0.2
benz[*a*]anthracene	0.4	0.4	0.1	0.4	0.3	-0.1	0.1	0.0	0.3
chrysene				0.8	0.7	0.1			
triphenylene				0.1	-0.5	-0.1			
benzo[*b*]fluoranthene	0.1	0.0	-0.1	0.1	-0.1	0.7	0.3	-0.2	0.0
benzo[*j*]fluoranthene	0.1	-1.3	-0.1	0.1	-1.3	0.4	0.4	-1.2	0.6
benzo[*k*]fluoranthene	0.0	0.0	-0.4	0.0	0.5	0.0	0.0	0.4	0.0
benzo[*e*]pyrene	0.2	0.3	-0.4	0.4	0.3	0.5	0.5	-0.2	-0.1
benzo[*a*]pyrene	0.2	0.3	0.0	0.2	0.5	0.0	0.0	0.2	-0.1
perylene	0.5	-1.5	-1.9	0.3	-1.7		0.0	-1.5	3.8
indeno[1,2,3-*cd*]pyrene	0.1	0.1	-0.5	0.0	0.3	-0.3	-0.2	-0.2	-0.3
benzo[*ghi*]perylene	0.2	0.6	0.0	0.1	0.2	0.2	-0.2	-0.3	-0.2
dibenz[*a,h*]anthracene	0.8	0.6		0.8	1.0				
dibenz[*a,c*]anthracene	-0.1	0.2		0.0	0.0		0.8	-0.2	
benzo[*b*]chrysene	0.5	-0.3		0.4	0.1		0.2	0.2	
coronene	0.1	0.1	-2.0	0.1	-0.2	-1.1	-0.6	-0.7	-1.2
dibenzo[*a,e*]pyrene	0.1	-0.2		-0.2			0.8	0.2	
9-nitroanthracene	0.0	-0.1							
1-nitropyrene	0.6	0.5	-1.7						
2-nitrofluoranthene	-0.6	0.0	-1.8						
7-nitrobenz[*a*]anthracene	-0.3								
9-fluoreneone									
antraquinone (9,10-AQ)									
benzanthrone									
benz[*a*]anthracene-7,12-dione									
n-C20	0.4	-0.1					-2.3	1.3	
n-C21									
n-C22	-0.9	-0.7					-1.2	0.5	
n-C23	0.1	0.3							
n-C24	-0.1	-0.5					1.8	1.2	
n-C25	-0.8	0.2							
n-C26	-0.7	-1.5					1.6	-1.0	
n-C27	-0.2	0.7							
n-C28	-0.7	1.3					1.5	-0.7	
n-C29	0.2	-0.8							
n-C30	0.0	0.5					1.3	0.0	
n-C31	0.4	-0.3							
n-C32	0.4	-0.6					0.6	5.0	
abb 20R Cholestane (Chiron#0602,27)	-0.2								
aaa 20R-Cholestane (Chiron#0622,27)	0.1	-1.9							
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	0.0	-0.5							
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)									
17a(H),21b(H)-Hopane (Chiron#0132,30)									
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)									
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)									
phytane	-0.9								
cholesterol									
hexadecanoic acid									
levoglucosan									

Table 5. Z-scores (25%) for data reported in Trial III

Laboratory No.	2			3a	3b	4	5	
	SRM 1648	Balt-2 PM	RM 8785	RM 8785	RM 8785	RM 8785	SRM 1648	Balt-2 PM
naphthalene	0.3	-1.5	39.5	-2.6	2.1			
fluorene	0.2	-1.0	5.6	-2.4	-2.6	-3.1		
phenanthrene	0.7	-0.8	4.1	-2.6	-2.6	4.9		
anthracene	0.3	-1.7	1.7	-2.8	-1.8	2.9		
1-methylphenanthrene					1.9			
2-methylphenanthrene					-0.7			
3-methylphenanthrene					-1.0			
9-methylphenanthrene					0.3			
retene								
4H-cyclopenta[*def*]phenanthrene								
fluoranthene	0.3	-0.3	2.6	-0.9	-1.5	0.6		
pyrene	0.0	-0.5	2.3	-1.4	-1.6	1.5		
benzo[*ghi*]fluoranthene								
cyclopenta[*cd*]pyrene								
benz[*a*]anthracene	0.6	-0.2	3.1	-1.5	-1.5	-0.2		
chrysene	0.5	-1.2	1.2	-0.5	-1.1	5.7		
triphenylene								
benzo[*b*]fluoranthene	0.6	-1.1		-0.3	-0.7	-1.0		
benzo[*j*]fluoranthene					-0.9			
benzo[*k*]fluoranthene	0.7	-0.8	2.0	-0.7	3.4	-1.1		
benzo[*e*]pyrene						-0.1		
benzo[*a*]pyrene	0.2	-0.9	1.7	-0.1	-1.9	0.3		
perylene						-1.9		
indeno[1,2,3-*cd*]pyrene	0.4	-1.0	1.7	-0.1	-0.8	-0.3		
benzo[*ghi*]perylene	0.0	-1.1	2.2	0.1	-1.3	-0.2		
dibenz[*a,h*]anthracene	-0.1	-1.3		-1.8	0.4	-2.2		
dibenz[*a,c*]anthracene								
benzo[*b*]chrysene								
coronene	0.0	-1.4	1.4					
dibenzo[*a,e*]pyrene								
9-nitroanthracene						0.2		
1-nitropyrene						3.3		
2-nitrofluoranthene						2.9		
7-nitrobenz[*a*]anthracene						0.8		
9-fluoreneone							-0.7	-0.7
antraquinone (9,10-AQ)							-0.5	-1.7
benzanthrone							-3.0	-2.0
benz[*a*]anthracene-7,12-dione							1.1	-1.0
n-C20						-2.2	-1.1	-2.6
n-C21						0.1	-1.7	-3.4
n-C22						-3.3	-1.6	-1.3
n-C23						-2.4	-0.8	-2.2
n-C24						-3.1	-0.1	-2.4
n-C25						-3.4	-0.6	-2.4
n-C26						-3.4	0.1	-2.8
n-C27						-3.8	-0.3	-2.2
n-C28						-3.4	0.3	-2.8
n-C29						-3.5	-0.4	-1.8
n-C30						-3.2	0.7	-2.7
n-C31						-3.4	0.3	-1.8
n-C32						-3.6	2.6	-3.2
abb 20R Cholestane (Chiron#0602,27)								
aaa 20R-Cholestane (Chiron#0622,27)								
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)								
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)								
17a(H),21b(H)-Hopane (Chiron#0132,30)								
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)								
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)								
phytane								
cholesterol							-1.3	-2.7
hexadecanoic acid							0.5	-1.3
levoglucosan							-2.3	-3.5

Table 5. Z-scores (25%) for data reported in Trial III

Laboratory No.	6		7			8	
	SRM 1648	Balt-2 PM	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM
naphthalene			56.6	126.3	1474.6	2.1	4.9
fluorene	-1.5	-2.5	0.0	3.1	10.9	0.3	-0.4
phenanthrene	-0.5	-2.2	-0.3	0.5	3.0	-0.8	2.3
anthracene	0.6		-1.0	0.4	5.0	-1.0	3.9
1-methylphenanthrene						0.0	3.4
2-methylphenanthrene						-0.8	4.2
3-methylphenanthrene						-0.6	1.8
9-methylphenanthrene						-0.5	3.5
retene			-0.5	-2.6		-2.6	-0.7
4H-cyclopenta[*def*]phenanthrene	4.4	5.7				-1.0	6.7
fluoranthene	0.4	-1.0	-0.5	0.0	0.0	-0.2	-2.8
pyrene	0.3	-0.9	-0.3	-0.5	0.6	-0.6	2.0
benzo[*ghi*]fluoranthene	4.7	-1.5	-0.6	-1.3	-0.2		
cyclopenta[*cd*]pyrene	13.0	0.0				-1.0	
benz[*a*]anthracene	3.3		0.2	0.1	1.3	1.7	3.2
chrysene			0.1	-0.6	0.0		
triphenylene			-0.3	-1.2	0.1		
benzo[*b*]fluoranthene			1.3	-0.1	1.2	0.0	2.7
benzo[*j*]fluoranthene						-0.6	3.8
benzo[*k*]fluoranthene						-0.5	7.9
benzo[*e*]pyrene	0.6	-2.0	0.1	-0.9	0.1	0.3	0.1
benzo[*a*]pyrene	0.7	-1.5	-0.2	-1.0		-1.0	-1.4
perylene	0.6		-0.3			-0.9	
indeno[1,2,3-*cd*]pyrene	1.4	0.8	0.3	-0.3	1.3		
benzo[*ghi*]perylene	0.0	-1.4	-0.5	-1.3	-0.1	0.7	3.4
dibenz[*a,h*]anthracene			1.6				
dibenz[*a,c*]anthracene						-0.6	
benzo[*b*]chrysene	0.0		-3.7			-1.1	
coronene	4.9	-0.3				0.8	1.1
dibenzo[*a,e*]pyrene	11.8					-0.6	
9-nitroanthracene			0.0	0.1	-0.2		
1-nitropyrene			-0.6	-0.5	-1.7		
2-nitrofluoranthene			0.6	0.0	-1.1		
7-nitrobenz[*a*]anthracene			0.3		-0.8		
9-fluoreneone							
antraquinone (9,10-AQ)							
benzanthrone							
benz[*a*]anthracene-7,12-dione							
n-C20							
n-C21							
n-C22							
n-C23							
n-C24							
n-C25							
n-C26							
n-C27							
n-C28							
n-C29							
n-C30							
n-C31							
n-C32							
abb 20R Cholestane (Chiron#0602,27)							
aaa 20R-Cholestane (Chiron#0622,27)							
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)							
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)							
17a(H),21b(H)-Hopane (Chiron#0132,30)							
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)							
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)							
phytane							
cholesterol							
hexadecanoic acid							
levoglucosan							

Table 5. Z-scores (25%) for data reported in Trial III

Laboratory No.	9			10a			10b	
	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785	Balt-2 PM	RM 8785
naphthalene	-1.5	-3.3	-2.1					
fluorene	-0.8	7.7	-2.6					
phenanthrene	0.0	-0.4	-2.7					
anthracene	1.9	1.7	-0.9					
1-methylphenanthrene	-1.0	-1.0	-0.6					
2-methylphenanthrene	-2.4	-2.4	-1.6					
3-methylphenanthrene								
9-methylphenanthrene								
retene	-0.6	6.2						
4H-cyclopenta[*def*]phenanthrene								
fluoranthene	0.0	0.6	-0.5					
pyrene	0.4	-0.1	-0.4					
benzo[*ghi*]fluoranthene								
cyclopenta[*cd*]pyrene								
benz[*a*]anthracene	-0.4	-0.6	0.8					
chrysene	0.5	-0.1	2.0					
triphenylene								
benzo[*b*]fluoranthene	-0.2	-0.8	1.7					
benzo[*j*]fluoranthene								
benzo[*k*]fluoranthene	-0.2	-0.1	1.6					
benzo[*e*]pyrene	1.8	0.8	31.9					
benzo[*a*]pyrene	0.7	1.9	6.7					
perylene								
indeno[1,2,3-*cd*]pyrene	-1.1	-0.4	1.2					
benzo[*ghi*]perylene	-0.7	-1.1	0.8					
dibenz[*a,h*]anthracene	-1.3	-0.2	6.5					
dibenz[*a,c*]anthracene								
benzo[*b*]chrysene								
coronene								
dibenzo[*a,e*]pyrene								
9-nitroanthracene								
1-nitropyrene								
2-nitrofluoranthene								
7-nitrobenz[*a*]anthracene								
9-fluoreneone								
antraquinone (9,10-AQ)								
benzanthrone								
benz[*a*]anthracene-7,12-dione								
n-C20	27.6	39.4	-1.3	-0.6		-1.8		
n-C21				0.2	-1.5	-0.1		
n-C22	-1.0	-1.3	-2.1	-0.5	0.5	-2.9		
n-C23				1.3	1.0	0.1		
n-C24		-2.2	-2.4	2.3	2.8	-0.3		
n-C25				1.0	2.4	0.5		
n-C26	-1.7	3.3	-2.9	1.8	0.5	1.2		
n-C27				1.5	1.2	-1.7		
n-C28	-1.5	1.6	-2.6	2.1	0.6	2.2		
n-C29				1.2	1.6	1.6		
n-C30	-1.6	1.7	-2.2	2.0	0.7	0.3		
n-C31				1.2	1.6	1.5		
n-C32	-1.1	0.2	-2.3	0.5	-1.2	-1.7		
abb 20R Cholestane (Chiron#0602,27)				0.2				
aaa 20R-Cholestane (Chiron#0622,27)				-0.1			1.9	
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)				-0.1	-0.6		1.0	
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)					0.2		-0.2	
17a(H),21b(H)-Hopane (Chiron#0132,30)				-1.7		-1.4		-0.5
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)				1.1				
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)				0.3				
phytane						-2.6		
cholesterol								
hexadecanoic acid								
levoglucosan								

Table 5. Z-scores (25%) for data reported in Trial 111

Laboratory No.	11			12			13		
	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785
naphthalene	2.6	7.1	217.5	-0.8	0.5	7.6			
fluorene	5.8	25.0	75.6						
phenanthrene	0.5	1.0	4.8	-2.0	-1.7	-2.1			
anthracene	4.2			0.6					
1-methylphenanthrene	3.9	7.3							
2-methylphenanthrene	0.6	-0.4							
3-methylphenanthrene	0.6								
9-methylphenanthrene	1.2								
retene									
4H-cyclopenta[*def*]phenanthrene									
fluoranthene	-0.4	0.6	4.3	-2.5	-2.4	-2.5			
pyrene	0.2	0.9	6.2	-2.5	-1.8	-2.5			
benzo[*ghi*]fluoranthene	5.8	10.3	38.4						
cyclopenta[*cd*]pyrene	4.6		37.6	1.1					
benz[*a*]anthracene	3.1	1.9	28.2	-2.2					
chrysene	-1.3	1.4	12.4	-3.1					
triphenylene	1.2	1.7	19.6	-1.0					
benzo[*b*]fluoranthene				-2.3			-1.1		
benzo[*j*]fluoranthene									
benzo[*k*]fluoranthene							3.2		
benzo[*e*]pyrene	-0.3	1.5	12.8	-2.1			-1.5		
benzo[*a*]pyrene	-0.3	1.8	26.1	-3.1					
perylene	-0.2	4.7	75.8						
indeno[1,2,3-*cd*]pyrene	0.2	1.1	14.0						
benzo[*ghi*]perylene	0.6	1.4	13.2	-2.4					
dibenz[*a,h*]anthracene									
dibenz[*a,c*]anthracene									
benzo[*b*]chrysene	1.3	30.6							
coronene	-0.4	1.4	2.9						
dibenzo[*a,e*]pyrene	0.8								
9-nitroanthracene									
1-nitropyrene									
2-nitrofluoranthene									
7-nitrobenz[*a*]anthracene									
9-fluoreneone	0.7	0.7							
antraquinone (9,10-AQ)	0.5	1.7							
benzanthrone	3.0	2.0							
benz[*a*]anthracene-7,12-dione	-1.1	1.0							
n-C20	-0.2	2.9	1.5	3.8	-1.4	3.9			
n-C21	3.1	6.1	40.3	-1.6	-1.2	0.0			
n-C22	1.6	23.3	3.7	3.6	2.3	4.6			
n-C23	8.9	44.1	36.8	-0.7	0.9	2.3			
n-C24	7.0	53.1	4.6	-0.6	0.3	3.8	-1.4	0.8	-2.5
n-C25	2.7	19.4	3.9	-2.2	-0.2	-1.0			
n-C26	1.4	2.6	2.0	-1.0	0.0	4.1	-1.5	-1.1	-0.9
n-C27	1.3	1.5	-1.8	-2.3	-1.2	7.3			
n-C28	0.7	0.3	2.9	0.0	0.5	11.6	-2.4	-0.7	0.8
n-C29	0.7	1.9	1.5	-1.7	-0.8	0.3			
n-C30	2.0	0.6	3.0	-1.9	-1.8	0.7	-2.5	1.1	1.4
n-C31	1.3	2.5	5.1	-3.1	-2.1	-3.2			
n-C32	0.7	-0.8	2.4	-1.1	-0.6	3.6	-2.7	1.1	1.6
abb 20R Cholestane (Chiron#0602,27)									
aaa 20R-Cholestane (Chiron#0622,27)									
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)							0.1		
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)									
17a(H),21b(H)-Hopane (Chiron#0132,30)				2.7		1.9	-1.0		
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)							-1.1		
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)							-0.3		
phytane	0.9	-0.6	1.0		0.6	1.5			
cholesterol	-3.2	-2.9	-2.4	4.5	5.6	2.4			
hexadecanoic acid	1.8	2.6	2.3	-2.3	-1.2	-2.3			
levoglucosan	-0.6	0.6	1.2	2.9	2.9	-1.2			

Table 5. Z-scores (25%) for data reported in Trial III

Laboratory No.	14		
SRM	SRM 1648	Balt-2 PM	RM 8785
naphthalene	-2.7	-2.4	-0.8
fluorene	0.7	-1.8	
phenanthrene	-0.8	-0.1	-0.9
anthracene	-0.2	-1.2	-0.8
1-methylphenanthrene			
2-methylphenanthrene			
3-methylphenanthrene			
9-methylphenanthrene			
retene			
4H-cyclopenta[*def*]phenanthrene			
fluoranthene	-0.6	0.7	-0.9
pyrene	-0.7	0.0	-0.8
benzo[*ghi*]fluoranthene			
cyclopenta[*cd*]pyrene			
benz[*a*]anthracene	-1.0	0.0	-1.5
chrysene	-0.5	-0.2	-1.3
triphenylene			
benzo[*b*]fluoranthene	-1.1	-0.5	-1.4
benzo[*j*]fluoranthene			
benzo[*k*]fluoranthene	-0.6	0.0	-1.1
benzo[*e*]pyrene			
benzo[*a*]pyrene	-0.5	0.0	-1.8
perylene			
indeno[1,2,3-*cd*]pyrene	-1.0	-0.3	-1.7
benzo[*ghi*]perylene	-0.3	-0.4	-1.5
dibenz[*a,h*]anthracene	-0.2	-0.2	-0.6
dibenz[*a,c*]anthracene			
benzo[*b*]chrysene			
coronene			
dibenzo[*a,e*]pyrene			
9-nitroanthracene			
1-nitropyrene			
2-nitrofluoranthene			
7-nitrobenz[*a*]anthracene			
9-fluoreneone			
antraquinone (9,10-AQ)			
benzanthrone			
benz[*a*]anthracene-7,12-dione			
n-C20			
n-C21			
n-C22			
n-C23			
n-C24			
n-C25			
n-C26			
n-C27			
n-C28			
n-C29			
n-C30			
n-C31			
n-C32			
abb 20R Cholestane (Chiron#0602,27)			
aaa 20R-Cholestane (Chiron#0622,27)			
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)			
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)			
17a(H),21b(H)-Hopane (Chiron#0132,30)			
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)			
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)			
phytane			
cholesterol			
hexadecanoic acid			
levoglucosan			

Table 6. Z-scores (s) for data reported in Trial III

Laboratory No.	1a			1b			1c		
	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785
naphthalene	0.6	-0.5	-0.7				-0.6	-0.8	0.3
fluorene	0.6	-0.3	-0.7	1.2	-0.6		-0.4	-0.7	-0.4
phenanthrene	1.2	0.7	-0.5	1.2	0.4	-0.5	0.8	-0.1	-0.3
anthracene	-0.1	-0.6	-0.9	0.0	-0.6		-0.5	-0.4	0.2
1-methylphenanthrene	0.5	-0.5	-1.0	0.7	-0.5	-0.8	0.7	-0.3	1.0
2-methylphenanthrene	0.3	-0.5	-0.8	0.2	-0.5	-0.2	-0.3	-0.6	1.4
3-methylphenanthrene	0.2	-0.8	-0.8	-0.1	-0.5	0.1	-0.1	-0.3	1.4
9-methylphenanthrene	-0.1	-0.5	-0.7	-0.4	-0.5	-0.8	-0.5	-0.4	1.3
retene	1.0	-0.4		0.9	-0.4				
4H-cyclopenta[*def*]phenanthrene	0.5	-0.5		0.7	-0.5		0.3	-0.5	
fluoranthene	0.8	1.3	-0.1	1.0	1.1	-0.2	0.8	0.4	-0.1
pyrene	1.0	0.6	-0.4	0.9	0.6	-0.6	0.2	-0.3	-0.1
benzo[*ghi*]fluoranthene	0.9	0.2	0.5	0.7	0.1	0.6	-0.2	1.1	47.1
cyclopenta[*cd*]pyrene	0.4	1.0		0.0	0.4	-0.7	-0.5	-1.4	0.7
benz[*a*]anthracene	0.4	1.3	0.1	0.4	0.9	-0.1	0.1	0.0	0.2
chrysene				1.0	0.8	0.0			
triphenylene				0.2	-0.3	-0.7			
benzo[*b*]fluoranthene	0.1	0.0	-0.1	0.2	-0.1	0.7	0.3	-0.2	0.0
benzo[*j*]fluoranthene	0.3	-0.5	-0.2	0.2	-0.5	0.5	0.9	-0.5	1.0
benzo[*k*]fluoranthene	0.0	0.0	-0.4	0.0	1.1	0.0	0.1	0.8	0.0
benzo[*e*]pyrene	0.2	0.3	-1.2	0.4	0.3	1.5	0.5	-0.2	-0.3
benzo[*a*]pyrene	0.4	0.3	0.0	0.4	0.4	0.0	-0.1	0.2	-0.1
perylene	1.0	-0.5	-0.6	0.6	-0.5		0.1	-0.5	1.2
indeno[1,2,3-*cd*]pyrene	0.1	0.1	-0.5	0.1	0.4	-0.3	-0.3	-0.3	-0.3
benzo[*ghi*]perylene	0.5	0.4	0.0	0.3	0.1	0.2	-0.4	-0.2	-0.2
dibenz[*a,h*]anthracene	0.9	0.7		0.9	1.1				
dibenz[*a,c*]anthracene	-0.2	1.0		0.0	-0.1		1.3	-1.0	
benzo[*b*]chrysene	0.8	-1.1		0.6	0.3		0.3	0.8	
coronene	0.1	0.1	-1.0	0.2	-0.2	-0.5	-1.3	-0.7	-0.6
dibenzo[*a,e*]pyrene	0.1	-0.7		-0.4			1.3	0.7	
9-nitroanthracene	-0.7	-0.7							
1-nitropyrene	0.7	0.7	-0.6						
2-nitrofluoranthene	-0.7	-0.7	-0.7						
7-nitrobenz[*a*]anthracene	-0.7								
9-fluoreneone									
antraquinone (9,10-AQ)									
benzanthrone									
benz[*a*]anthracene-7,12-dione									
n-C20	0.2	-0.1					-1.1	0.6	
n-C21									
n-C22	-0.5	-0.5					-0.7	0.4	
n-C23	0.1	0.2							
n-C24	-0.1	-0.2					1.2	0.6	
n-C25	-0.4	0.1							
n-C26	-0.5	-0.7					1.1	-0.5	
n-C27	-0.2	0.4							
n-C28	-0.4	0.9					1.0	-0.5	
n-C29	0.2	-0.5							
n-C30	0.0	0.3					0.7	0.0	
n-C31	0.2	-0.1							
n-C32	0.2	-0.3					0.4	2.1	
abb 20R Cholestane (Chiron#0602,27)									
aaa 20R-Cholestane (Chiron#0622,27)									
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	0.3	-0.5							
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)									
17a(H),21b(H)-Hopane (Chiron#0132,30)									
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)									
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)									
phytane	-0.7								
cholesterol									
hexadecanoic acid									
levoglucosan									

Table 6. Z-scores (s) for data reported in Trial III

Laboratory No.	2			3a	3b	4	5	
	SRM 1648	Balt-2 PM	RM 8785	RM 8785	RM 8785	RM 8785	SRM 1648	Balt-2 PM
naphthalene	0.2	-0.4	10.1	-0.7	0.5			
fluorene	0.3	-0.3	1.1	-0.5	-0.5	-0.6		
phenanthrene	0.7	-0.6	1.3	-0.8	-0.8	1.5		
anthracene	0.4	-0.9	0.6	-1.0	-0.7	1.1		
1-methylphenanthrene					1.1			
2-methylphenanthrene					-0.4			
3-methylphenanthrene					-0.6			
9-methylphenanthrene					0.2			
retene								
4H-cyclopenta[*def*]phenanthrene								
fluoranthene	0.8	-0.2	1.4	-0.5	-0.8	0.3		
pyrene	-0.1	-0.5	1.0	-0.6	-0.7	0.6		
benzo[*ghi*]fluoranthene								
cyclopenta[*cd*]pyrene								
benz[*a*]anthracene	0.5	-0.7	2.0	-1.0	-1.0	-0.1		
chrysene	0.6	-1.3	1.0	-0.4	-0.8	4.5		
triphenylene								
benzo[*b*]fluoranthene	0.8	-0.9		-0.3	-0.6	-1.0		
benzo[*j*]fluoranthene					-1.3			
benzo[*k*]fluoranthene	1.7	-1.8	1.7	-0.5	2.8	-1.0		
benzo[*e*]pyrene						-0.2		
benzo[*a*]pyrene	0.4	-0.7	1.6	-0.1	-1.8	0.3		
perylene						-0.6		
indeno[1,2,3-*cd*]pyrene	0.5	-1.6	1.6	-0.1	-0.7	-0.3		
benzo[*ghi*]perylene	0.0	-0.7	2.1	0.1	-1.3	-0.2		
dibenz[*a,h*]anthracene	-0.1	-1.5		-0.4	0.1	-0.5		
dibenz[*a,c*]anthracene								
benzo[*b*]chrysene								
coronene	0.1	-1.4	0.7					
dibenzo[*a,e*]pyrene								
9-nitroanthracene						0.7		
1-nitropyrene						1.2		
2-nitrofluoranthene						1.1		
7-nitrobenz[*a*]anthracene						0.7		
9-fluoreneone							-0.7	-0.7
antraquinone (9,10-AQ)							-0.7	-0.7
benzanthrone							-0.7	-0.7
benz[*a*]anthracene-7,12-dione							0.7	-0.7
n-C20						-0.9	-0.5	-1.2
n-C21						1.0	-0.8	-0.8
n-C22						-0.9	-0.8	-0.9
n-C23						-1.0	-0.8	-1.5
n-C24						-0.9	-0.1	-1.3
n-C25						-1.1	-0.3	-1.2
n-C26						-1.2	0.1	-1.4
n-C27						-0.8	-0.2	-1.3
n-C28						-1.2	0.2	-2.0
n-C29						-1.5	-0.4	-1.1
n-C30						-1.4	0.4	-1.8
n-C31						-0.8	0.2	-0.9
n-C32						-1.2	1.7	-1.3
abb 20R Cholestane (Chiron#0602,27)								
aaa 20R-Cholestane (Chiron#0622,27)								
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)								
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)								
17a(H),21b(H)-Hopane (Chiron#0132,30)								
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)								
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)								
phytane								
cholesterol							-0.3	-0.6
hexadecanoic acid							0.2	-0.6
levoglucosan							-0.9	-1.1

Table 6. Z-scores (s) for data reported in Trial III

Laboratory No.	6		7			8	
	SRM 1648	Balt-2 PM	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM
naphthalene			30.7	32.1	375.2	1.1	1.3
fluorene	-2.0	-0.7	0.0	0.9	2.0	0.4	-0.1
phenanthrene	-0.5	-1.7	-0.3	0.4	0.9	-0.8	1.8
anthracene	0.6		-1.2	0.2	1.8	-1.2	2.0
1-methylphenanthrene						-0.1	1.8
2-methylphenanthrene						-1.5	1.8
3-methylphenanthrene						-1.4	1.5
9-methylphenanthrene						-0.7	1.5
retene			-0.3	-0.7		-1.4	-0.2
4H-cyclopenta[*def*]phenanthrene	6.6	1.3				-1.5	1.5
fluoranthene	0.9	-0.6	-1.2	0.0	0.0	-0.4	-1.8
pyrene	0.6	-0.9	-0.7	-0.5	0.2	-1.5	2.0
benzo[*ghi*]fluoranthene	10.7	-1.5	-1.3	-1.3	-1.2		
cyclopenta[*cd*]pyrene	16.7	0.0				-1.3	
benz[*a*]anthracene	3.0		0.2	0.2	0.8	1.6	9.9
chrysene			0.1	-0.6	0.0		
triphenylene			-0.3	-0.8	0.7		
benzo[*b*]fluoranthene			1.7	-0.1	1.2	0.0	2.3
benzo[*j*]fluoranthene						-1.4	1.5
benzo[*k*]fluoranthene						-1.3	17.3
benzo[*e*]pyrene	0.5	-1.9	0.1	-0.8	0.2	0.3	0.1
benzo[*a*]pyrene	1.4	-1.2	-0.4	-0.8		-1.8	-1.1
perylene	1.1		-0.7			-1.7	
indeno[1,2,3-*cd*]pyrene	1.9	1.2	0.4	-0.5	1.2		
benzo[*ghi*]perylene	0.0	-0.9	-1.1	-0.9	-0.1	1.5	2.3
dibenz[*a,h*]anthracene			1.8				
dibenz[*a,c*]anthracene						-1.1	
benzo[*b*]chrysene	0.0		-5.9			-1.7	
coronene	10.6	-0.3				1.6	1.1
dibenzo[*a,e*]pyrene	20.6					-1.1	
9-nitroanthracene			0.7	0.7	-0.7		
1-nitropyrene			-0.7	-0.7	-0.6		
2-nitrofluoranthene			0.7	0.7	-0.4		
7-nitrobenz[*a*]anthracene			0.7		-0.7		
9-fluoreneone							
antraquinone (9,10-AQ)							
benzanthrone							
benz[*a*]anthracene-7,12-dione							
n-C20							
n-C21							
n-C22							
n-C23							
n-C24							
n-C25							
n-C26							
n-C27							
n-C28							
n-C29							
n-C30							
n-C31							
n-C32							
abb 20R Cholestane (Chiron#0602,27)							
aaa 20R-Cholestane (Chiron#0622,27)							
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)							
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)							
17a(H),21b(H)-Hopane (Chiron#0132,30)							
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)							
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)							
phytane							
cholesterol							
hexadecanoic acid							
levoglucosan							

Table 6. Z-scores (s) for data reported in Trial III

Laboratory No.	9			10a			10b	
	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785	Balt-2 PM	RM 8785
naphthalene	-0.8	-0.8	-0.5					
fluorene	-1.0	2.3	-0.5					
phenanthrene	0.0	-0.3	-0.9					
anthracene	2.1	0.9	-0.3					
1-methylphenanthrene	-1.7	-0.5	-0.3					
2-methylphenanthrene	-4.7	-1.0	-0.9					
3-methylphenanthrene								
9-methylphenanthrene								
retene	-0.3	1.8						
4H-cyclopenta[*def*]phenanthrene								
fluoranthene	-0.1	0.4	-0.3					
pyrene	0.9	-0.1	-0.2					
benzo[*ghi*]fluoranthene								
cyclopenta[*cd*]pyrene								
benz[*a*]anthracene	-0.3	-1.8	0.5					
chrysene	0.7	-0.1	1.6					
triphenylene								
benzo[*b*]fluoranthene	-0.2	-0.7	1.6					
benzo[*j*]fluoranthene								
benzo[*k*]fluoranthene	-0.4	-0.1	1.3					
benzo[*e*]pyrene	1.6	0.8	97.3					
benzo[*a*]pyrene	1.3	1.6	6.4					
perylene								
indeno[1,2,3-*cd*]pyrene	-1.4	-0.6	1.1					
benzo[*ghi*]perylene	-1.6	-0.7	0.7					
dibenz[*a,h*]anthracene	-1.5	-0.2	1.5					
dibenz[*a,c*]anthracene								
benzo[*b*]chrysene								
coronene								
dibenzo[*a,e*]pyrene								
9-nitroanthracene								
1-nitropyrene								
2-nitrofluoranthene								
7-nitrobenz[*a*]anthracene								
9-fluoreneone								
antraquinone (9,10-AQ)								
benzanthrone								
benz[*a*]anthracene-7,12-dione								
n-C20	13.3	18.3	-0.5	-0.3		-0.7		
n-C21				0.1	-0.4	-1.0		
n-C22	-0.5	-0.9	-0.5	-0.3	0.4	-0.8		
n-C23				1.4	0.7	0.0		
n-C24	-1.2	-1.2	-0.7	1.5	1.5	-0.1		
n-C25				0.5	1.2	0.2		
n-C26	-1.2	1.6	-1.0	1.3	0.2	0.4		
n-C27				1.0	0.8	-0.3		
n-C28	-1.0	1.1	-0.9	1.4	0.4	0.8		
n-C29				1.1	1.0	0.7		
n-C30	-0.9	1.2	-1.0	1.1	0.4	0.1		
n-C31				0.7	0.8	0.4		
n-C32	-0.7	0.1	-0.8	0.3	-0.5	-0.6		
abb 20R Cholestane (Chiron#0602,27)				0.7				
aaa 20R-Cholestane (Chiron#0622,27)				-0.7			0.7	
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)				-1.1	-0.6		1.2	
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)					0.7		-0.7	
17a(H),21b(H)-Hopane (Chiron#0132,30)				-0.7		-0.8		-0.3
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)				0.7				
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)				0.7				
phytane						-1.1		
cholesterol								
hexadecanoic acid								
levoglucosan								

Table 6. Z-scores (s) for data reported in Trial III

Laboratory No.	11			12			13		
	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785	SRM 1648	Balt-2 PM	RM 8785
naphthalene	1.4	1.8	55.3	-0.4	0.1	1.9			
fluorene	7.6	7.5	14.3						
phenanthrene	0.5	0.8	1.5	-2.0	-1.3	-0.6			
anthracene	4.8			0.7					
1-methylphenanthrene	6.6	3.8							
2-methylphenanthrene	1.2	-0.2							
3-methylphenanthrene	1.4								
9-methylphenanthrene	1.7								
retene									
4H-cyclopenta[*def*]phenanthrene									
fluoranthene	-1.1	0.4	2.3	-6.0	-1.6	-1.4			
pyrene	0.5	0.8	2.6	-6.0	-1.8	-1.0			
benzo[*ghi*]fluoranthene	13.2	10.3	249.8						
cyclopenta[*cd*]pyrene	6.0		143.1	1.4					
benz[*a*]anthracene	2.9	5.8	18.1	-2.0					
chrysene	-1.7	1.5	9.8	-4.0					
triphenylene	1.3	1.1	129.0	-1.1					
benzo[*b*]fluoranthene				-3.0			-1.4		
benzo[*j*]fluoranthene									
benzo[*k*]fluoranthene							7.6		
benzo[*e*]pyrene	-0.3	1.4	39.0	-1.9			-1.4		
benzo[*a*]pyrene	-0.7	1.5	25.2	-6.0					
perylene	-0.3	1.5	22.9						
indeno[1,2,3-*cd*]pyrene	0.2	1.7	13.0						
benzo[*ghi*]perylene	1.5	0.9	12.5	-5.4					
dibenz[*a,h*]anthracene									
dibenz[*a,c*]anthracene									
benzo[*b*]chrysene	2.0	119.8							
coronene	-0.8	1.4	1.4						
dibenzo[*a,e*]pyrene	1.4								
9-nitroanthracene									
1-nitropyrene									
2-nitrofluoranthene									
7-nitrobenz[*a*]anthracene									
9-fluoreneone	0.7	0.7							
antraquinone (9,10-AQ)	0.7	0.7							
benzanthrone	0.7	0.7							
benz[*a*]anthracene-7,12-dione	-0.7	0.7							
n-C20	-0.1	1.3	0.6	1.8	-0.7	1.5			
n-C21	1.4	1.5	438.8	-0.7	-0.3	0.0			
n-C22	0.9	16.4	1.0	1.9	1.6	1.2			
n-C23	9.1	28.8	15.5	-0.7	0.6	1.0			
n-C24	4.6	28.4	1.4	-0.4	0.2	1.1	-0.9	0.4	-0.8
n-C25	1.4	9.9	1.3	-1.2	-0.1	-0.3			
n-C26	0.9	1.3	0.7	-0.7	0.0	1.4	-1.0	-0.5	-0.3
n-C27	0.8	0.9	-0.4	-1.5	-0.8	1.5			
n-C28	0.5	0.2	1.0	0.0	0.4	4.1	-1.6	-0.5	0.3
n-C29	0.6	1.1	0.6	-1.5	-0.5	0.1			
n-C30	1.1	0.4	1.3	-1.1	-1.2	0.3	-1.4	0.7	0.6
n-C31	0.7	1.2	1.3	-1.7	-1.0	-0.8			
n-C32	0.5	-0.3	0.8	-0.7	-0.3	1.2	-1.7	0.5	0.5
abb 20R Cholestane (Chiron#0602,27)									
aaa 20R-Cholestane (Chiron#0622,27)									
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)					381.7		0.8		
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)									
17a(H),21b(H)-Hopane (Chiron#0132,30)				1.1		1.1	-0.4		
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)							-0.7		
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)							-0.7		
phytane	0.7	-0.7	0.5		0.7	0.7			
cholesterol	-0.8	-0.6	-0.7	1.1	1.2	0.7			
hexadecanoic acid	0.9	1.2	0.7	-1.1	-0.6	-0.7			
levoglucosan	-0.2	0.2	0.7	1.1	0.9	-0.7			

Table 6. Z-scores (s) for data reported in Trial III

Laboratory No.	14		
	SRM 1648	Balt-2 PM	RM 8785
naphthalene	-1.5	-0.6	-0.8
fluorene	0.9	-0.5	
phenanthrene	-0.8	-0.1	-0.9
anthracene	-0.2	-0.6	-0.8
1-methylphenanthrene			
2-methylphenanthrene			
3-methylphenanthrene			
9-methylphenanthrene			
retene			
4H-cyclopenta[*def*]phenanthrene			
fluoranthene	-1.5	0.5	-0.9
pyrene	-1.7	0.0	-0.8
benzo[*ghi*]fluoranthene			
cyclopenta[*cd*]pyrene			
benz[*a*]anthracene	-0.9	0.1	-1.5
chrysene	-0.7	-0.3	-1.3
triphenylene			
benzo[*b*]fluoranthene	-1.5	-0.4	-1.4
benzo[*j*]fluoranthene			
benzo[*k*]fluoranthene	-1.4	0.0	-1.1
benzo[*e*]pyrene			
benzo[*a*]pyrene	-0.9	0.0	-1.8
perylene			
indeno[1,2,3-*cd*]pyrene	-1.4	-0.5	-1.7
benzo[*ghi*]perylene	-0.7	-0.3	-1.5
dibenz[*a,h*]anthracene	-0.2	-0.2	-0.6
dibenz[*a,c*]anthracene			
benzo[*b*]chrysene			
coronene			
dibenzo[*a,e*]pyrene			
9-nitroanthracene			
1-nitropyrene			
2-nitrofluoranthene			
7-nitrobenz[*a*]anthracene			
9-fluoreneone			
antraquinone (9,10-AQ)			
benzanthrone			
benz[*a*]anthracene-7,12-dione			
n-C20			
n-C21			
n-C22			
n-C23			
n-C24			
n-C25			
n-C26			
n-C27			
n-C28			
n-C29			
n-C30			
n-C31			
n-C32			
abb 20R Cholestane (Chiron#0602,27)			
aaa 20R-Cholestane (Chiron#0622,27)			
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)			
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)			
17a(H),21b(H)-Hopane (Chiron#0132,30)			
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)			
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)			
phytane			
cholesterol			
hexadecanoic acid			
levoglucosan			

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	1a				1b			
	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a
naphthalene	0.03	0.34	0.41	0.28				
fluorene	0.43	0.35	0.33	0.32	0.74	0.30		0.45
phenanthrene	0.05	0.49	0.16	0.11	0.08	0.11		0.28
anthracene	0.24	0.26	0.29	0.30	0.23	0.44	1.74	0.43
1-methylphenanthrene	0.12	0.15	0.19	0.11	0.24	0.25		0.24
2-methylphenanthrene	0.29	0.37	0.06	0.31	0.11	0.09	1.99	0.03
3-methylphenanthrene	0.11	0.48	0.32	0.12	0.25	0.26	2.59	0.14
9-methylphenanthrene	0.42	0.38	0.21	0.20	0.23	0.31	2.21	0.17
retene	0.23	0.30	0.40	0.41	0.16	0.61	3.96	0.17
4H-cyclopenta[*def*]phenanthrene	0.27	0.38	0.37	0.28	0.15	0.22		0.29
fluoranthene	0.06	0.17	0.76	0.15	0.16	0.05		0.26
pyrene	0.15	0.14	0.29	0.06	0.09	0.06	1.10	0.27
benzo[*ghi*]fluoranthene	0.24	0.12	0.33	0.31	0.03	0.05	1.61	0.08
cyclopenta[*cd*]pyrene	0.12	0.22		0.25	0.07	0.26	1.59	0.27
benz[*a*]anthracene	0.14	0.29	0.39	0.12	0.04	0.06	0.71	0.37
chrysene					0.11	0.05	0.89	0.21
triphenylene					0.09	0.14	0.58	0.09
benzo[*b*]fluoranthene	0.06	0.30	0.53	0.14	0.09	0.07	0.87	0.14
benzo[*j*]fluoranthene	0.14	0.15	0.62	0.05	0.08	0.05	0.74	0.21
benzo[*k*]fluoranthene	0.11	0.23	0.70	0.18	0.12	0.17	0.57	0.28
benzo[*e*]pyrene	0.18	0.20	0.72	0.15	0.07	0.02	1.00	0.17
benzo[*a*]pyrene	0.34	0.30	0.74	0.36	0.14	0.07	0.66	0.26
perylene	0.30	0.22	0.94	0.24	0.07	0.24	1.27	0.32
indeno[1,2,3-*cd*]pyrene	0.16	0.13	0.42	0.10	0.12	0.13		0.24
benzo[*ghi*]perylene	0.11	0.31	0.44	0.10	0.08	0.02	0.74	0.15
dibenz[*a,h*]anthracene	0.15	0.29		0.82	0.26	0.45	0.52	0.70
dibenz[*a,c*]anthracene	0.57	0.31		0.36	0.43	0.33		0.41
benzo[*b*]chrysene	0.20	0.25		0.31	0.23	0.46		0.52
coronene	0.56	0.23	0.36	0.39	0.04	0.13		0.18
dibenzo[*a,e*]pyrene	0.38	0.90		0.06	0.11		0.83	0.45
9-nitroanthracene	0.32	0.65		0.21				
1-nitropyrene	0.09	0.63	0.72	0.22				
2-nitrofluoranthene	1.68	0.58	0.30	0.29				
3-nitrofluoranthene	0.91			0.08				
7-nitrobenz[*a*]anthracene	0.46			0.74				
6-nitrochrysene								
6-nitrobenzo[*a*]pyrene								
9-fluoreneone								
acenaphthenequinone								
perinaphthenone								
antraquinone (9,10-AQ)								
benzanthrone								
benz[*a*]anthracene-7,12-dione								
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one								
n-C20	0.20	0.47	0.56	0.48				
n-C21								
n-C22	0.09	0.29		0.40				
n-C23	0.27	0.30		0.40				
n-C24	0.13	0.86		0.51				
n-C25	0.15	0.39		0.26				
n-C26	0.26	0.19		0.41				
n-C27	0.02	0.21		0.15				
n-C28	0.24	0.20		0.97				
n-C29	0.19	0.52		0.42				
n-C30	0.37	0.29		0.14				
n-C31	0.30	0.24		0.47				
n-C32	0.13	0.23		0.37				
n-C40								
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)								
abb 20R 24R-Ethylcholestane (Chiron#0662,29)								
abb 20R 24S-Methylcholestane (Chiron#0643,28)								
abb 20R Cholestane (Chiron#0602,27)	0.36			0.24				
aaa 20R-Cholestane (Chiron#0622,27)	0.31	0.44		0.16				
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	0.26	1.00		0.56				
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)								
17a(H),21b(H)-Hopane (Chiron#0132,30)								
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)								
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)								
pristane								
phytane	0.55			0.39				
cholesterol								
stigmasterol								
pimaric acid								
isopimaric acid								
pinonic acid								
hexadecanoic acid								
syringol								
isoeugenol								
levoglucosan								

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	1c				2			
	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a
naphthalene	0.19	1.43	1.84		0.93	3.54	5.89	0.72
fluorene	0.32	0.50	1.60		1.77	0.11	3.61	0.44
phenanthrene	0.06	0.50	1.25		0.59	0.88	2.39	0.27
anthracene	0.19	0.71	1.75	0.12	1.62	0.97	2.51	0.41
1-methylphenanthrene	0.07	0.16	1.95					
2-methylphenanthrene	0.06	0.34	1.24	0.13				
3-methylphenanthrene	0.10	0.45	1.52	0.17				
9-methylphenanthrene	0.10	0.25	1.48	0.15				
retene	0.00	0.00	0.00	0.26				
4H-cyclopenta[*def*]phenanthrene	0.10	0.42	1.51					
fluoranthene	0.09	0.34	1.28		0.55	0.17	1.53	0.25
pyrene	0.20	0.31	1.26	0.07	0.49	0.13	1.37	0.31
benzo[*ghi*]fluoranthene	0.07	0.63	2.08	0.11				
cyclopenta[*cd*]pyrene	0.21	0.52	1.22	0.11				
benz[*a*]anthracene	0.12	0.39	1.36	0.05	0.43	0.17	1.26	0.17
chrysene	0.09	0.20	0.87	0.06	0.53	0.26	1.04	0.24
triphenylene				0.04				
benzo[*b*]fluoranthene	0.19	0.25	0.42	0.06	0.36	0.28	1.02	0.17
benzo[*j*]fluoranthene	0.11	0.25	0.66	0.05				
benzo[*k*]fluoranthene	0.21	0.34	0.67	0.04	0.87	0.33	1.29	0.17
benzo[*e*]pyrene	0.21	0.20	0.59	0.07				
benzo[*a*]pyrene	0.21	0.14	1.24	0.04	0.66	0.50	1.49	0.33
perylene	0.20	0.88	2.22	0.08				
indeno[1,2,3-*cd*]pyrene	0.10	0.16	0.73	0.00	0.72	0.58	1.25	0.38
benzo[*ghi*]perylene	0.12	0.08	0.55	0.05	0.76	0.28	1.17	0.28
dibenz[*a,h*]anthracene				0.03	0.98	0.52		0.23
dibenz[*a,c*]anthracene	0.48	0.29						
benzo[*b*]chrysene	0.04	0.10	1.09					
coronene	0.29	0.55	0.46		0.27	0.60	1.25	0.57
dibenzo[*a,e*]pyrene	0.19	0.08		0.06				
9-nitroanthracene								
1-nitropyrene								
2-nitrofluoranthene								
3-nitrofluoranthene								
7-nitrobenz[*a*]anthracene								
6-nitrochrysene								
6-nitrobenzo[*a*]pyrene								
9-fluoreneone								
acenaphthenequinone								
perinaphthenone								
antraquinone (9,10-AQ)								
benzanthrone								
benz[*a*]anthracene-7,12-dione								
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one								
n-C20	2.69	0.79		0.35				
n-C21								
n-C22	0.48	0.80		1.12				
n-C23								
n-C24	0.14	0.30		0.98				
n-C25								
n-C26	0.13	0.41		0.15				
n-C27								
n-C28	0.18	0.45		0.99				
n-C29								
n-C30	0.34	0.85		1.66				
n-C31								
n-C32	0.81	0.17		1.69				
n-C40								
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)								
abb 20R 24R-Ethylcholestane (Chiron#0662,29)								
abb 20R 24S-Methylcholestane (Chiron#0643,28)								
abb 20R Cholestane (Chiron#0602,27)								
aaa 20R-Cholestane (Chiron#0622,27)								
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)								
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)								
17a(H),21b(H)-Hopane (Chiron#0132,30)								
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)								
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)								
pristane								
phytane								
cholesterol								
stigmasterol								
pimaric acid								
isopimaric acid								
pinonic acid								
hexadecanoic acid								
syringol								
isoeugenol								
levoglucosan								

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	3a		3b		4		5		
	RM 8785	SRM 1649a	RM 8785	SRM 1649a	RM 8785	SRM 1649a	SRM 1648	Bait-2 PM	SRM 1649a
naphthalene	2.85	0.13	4.42	1.33					
fluorene	4.25	1.31		0.22	2.24	1.59			
phenanthrene	3.17	1.92	1.69	0.21	2.33	0.29			
anthracene	3.00	1.56	1.11	0.17	3.63	0.47			
1-methylphenanthrene			2.46	0.48					
2-methylphenanthrene			1.67	0.45					
3-methylphenanthrene			2.05	0.57					
9-methylphenanthrene			1.57	0.48					
retene									
4H-cyclopenta[*def*]phenanthrene									
fluoranthene	1.52	0.62	1.58	0.09	3.15	0.20			
pyrene	2.62	1.28	1.56	0.16	2.84	0.25			
benzo[*ghi*]fluoranthene									
cyclopenta[*cd*]pyrene									
benz[*a*]anthracene	1.87	0.81	1.37	0.21	2.29	0.23			
chrysene	1.18	0.73	1.33	0.23	3.40	2.54			
triphenylene									
benzo[*b*]fluoranthene	1.44	0.56	1.55	0.14	2.73	0.20			
benzo[*j*]fluoranthene			1.36	0.26					
benzo[*k*]fluoranthene	1.21	0.68	1.31	0.40	1.14	1.26			
benzo[*e*]pyrene					2.33	0.15			
benzo[*a*]pyrene	1.29	0.72	1.38	0.17	2.50	0.36			
perylene					3.17	0.41			
indeno[1,2,3-*cd*]pyrene	1.35	0.94	1.48	0.24	2.86	0.31			
benzo[*ghi*]perylene	1.04	0.61	1.46	0.37	2.76	0.26			
dibenz[*a,h*]anthracene	1.53	0.96	1.15	0.33	4.60	0.49			
dibenz[*a,c*]anthracene									
benzo[*b*]chrysene									
coronene									
dibenzo[*a,e*]pyrene									
9-nitroanthracene					3.30	0.08			
1-nitropyrene					2.95	0.18			
2-nitrofluoranthene					3.99	0.78			
3-nitrofluoranthene					4.08	2.01			
7-nitrobenz[*a*]anthracene					6.49	0.33			
6-nitrochrysene					4.39	3.80			
6-nitrobenzo[*a*]pyrene						3.55			
9-fluoreneone							0.66	1.58	2.19
acenaphthenequinone									
perinaphthenone									
anthraquinone (9,10-AQ)							0.67	4.24	0.99
benzanthrone							1.48	1.18	1.62
benz[*a*]anthracene-7,12-dione							0.24	4.11	0.23
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one									
n-C20					9.09	4.03	1.23	1.38	0.79
n-C21					9.04	3.01	0.70	2.53	1.97
n-C22					7.28	2.01	0.26	1.10	0.61
n-C23					6.73	1.08	0.11	0.59	0.44
n-C24					3.22	0.57	0.28	0.92	0.09
n-C25					1.96	0.62	0.35	0.22	0.21
n-C26					1.57	0.76	0.23	0.99	0.12
n-C27					1.52	0.85	0.21	0.74	0.32
n-C28					2.19	0.60	0.45	0.53	0.31
n-C29					2.13	0.84	0.53	1.00	0.32
n-C30					3.59	0.14	0.56	0.79	0.28
n-C31					3.23	0.91	0.34	1.09	0.50
n-C32					3.89	1.36	1.19	1.33	1.10
n-C40									
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)									
abb 20R 24R-Ethylcholestane (Chiron#0662,29)									
abb 20R 24S-Methylcholestane (Chiron#0643,28)									
abb 20R Cholestane (Chiron#0602,27)									
aaa 20R-Cholestane (Chiron#0622,27)									
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)									
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)									
17a(H),21b(H)-Hopane (Chiron#0132,30)									
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)									
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)									
pristane									
phytane									
cholesterol							0.64	0.31	0.66
stigmasterol									
pimaric acid									
isopimaric acid									
pinonic acid									
hexadecanoic acid							0.30	1.13	0.25
syringol									
isoeugenol									
levoglucosan							0.69	1.18	0.10

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	6			7			
	SRM 1648	Balt-2 PM	SRM 1649a	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a
naphthalene				0.55	0.52	3.19	0.56
fluorene	0.36	3.36	1.65	0.52	0.47	3.06	0.52
phenanthrene	0.40	0.31	0.33	0.44	0.51	2.65	0.68
anthracene	0.95		0.24	0.39	0.32	2.74	0.99
1-methylphenanthrene							
2-methylphenanthrene							
3-methylphenanthrene							
9-methylphenanthrene							
retene				0.23	0.42		0.24
4H-cyclopenta[*def*]phenanthrene	0.61	1.50	0.70				
fluoranthene	0.26	1.25	0.27	0.29	0.60	1.49	0.50
pyrene	0.34	0.57	0.34	0.26	0.49	1.79	0.59
benzo[*ghi*]fluoranthene	1.59	4.09	1.71	0.23	0.67	1.20	0.51
cyclopenta[*cd*]pyrene	1.38	4.13	3.49				
benz[*a*]anthracene	2.53		2.40	0.34	0.43	2.51	0.58
chrysene				0.36	0.45	0.88	0.44
triphenylene				0.35	0.57	1.10	0.28
benzo[*b*]fluoranthene				0.38	0.48	0.83	0.35
benzo[*j*]fluoranthene				0.39	0.58		0.43
benzo[*k*]fluoranthene				0.39	0.58		0.43
benzo[*e*]pyrene	0.38	0.09	0.35	0.38	0.51	1.00	0.36
benzo[*a*]pyrene	0.88	0.21	0.23	0.31	0.37		0.57
perylene	1.02		0.62	0.30			0.55
indeno[1,2,3-*cd*]pyrene	0.61	0.75	0.38	0.34	0.39	1.64	0.48
benzo[*ghi*]perylene	0.48	0.12	0.54	0.37	0.47	0.94	0.36
dibenz[*a,h*]anthracene				0.38			0.51
dibenz[*a,c*]anthracene							
benzo[*b*]chrysene	1.92		1.28	0.32			0.63
coronene	0.55	1.03	1.76				
dibenzo[*a,e*]pyrene	0.97		2.20				
9-nitroanthracene				0.11	0.61	0.94	0.26
1-nitropyrene				0.23	0.76	1.22	0.46
2-nitrofluoranthene				0.41	0.76	0.48	0.40
3-nitrofluoranthene							
7-nitrobenz[*a*]anthracene				0.11		2.18	0.76
6-nitrochrysene							
6-nitrobenzo[*a*]pyrene				0.70			0.41
9-fluoreneone							
acenaphthenequinone							
perinaphthenone							
antraquinone (9,10-AQ)							
benzanthrone							
benz[*a*]anthracene-7,12-dione							
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one							
n-C20							
n-C21							
n-C22							
n-C23							
n-C24							
n-C25							
n-C26							
n-C27							
n-C28							
n-C29							
n-C30							
n-C31							
n-C32							
n-C40							
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)							
abb 20R 24R-Ethylcholestane (Chiron#0662,29)							
abb 20R 24S-Methylcholestane (Chiron#0643,28)							
abb 20R Cholestane (Chiron#0602,27)							
aaa 20R-Cholestane (Chiron#0622,27)							
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)							
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)							
17a(H),21b(H)-Hopane (Chiron#0132,30)							
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)							
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)							
pristane							
phytane							
cholesterol							
stigmasterol							
pimaric acid							
isopimaric acid							
pinonic acid							
hexadecanoic acid							
syringol							
isoeugenol							
levoglucosan							

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	8			9			
	SRM 1648	Balt-2 PM	SRM 1649a	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a
naphthalene	0.89	1.03	0.35	1.27	0.33	5.14	0.49
fluorene	0.44	0.81	1.00	0.75	0.69		0.43
phenanthrene	0.20	0.42	0.29	0.60	0.63	2.75	0.69
anthracene	0.40	0.44	0.33	0.57	0.48	4.61	0.64
1-methylphenanthrene	0.16	0.71	0.37	2.34	0.93	1.28	0.10
2-methylphenanthrene	0.18	0.16	0.65	2.52	1.01	1.14	0.33
3-methylphenanthrene	0.13	0.44	0.15				
9-methylphenanthrene	0.20	0.43	0.34				
retene	0.42	0.89	0.89	2.48	0.40	4.41	0.12
4H-cyclopenta[*def*]phenanthrene	0.18	0.13	0.19				
fluoranthene	0.27	0.29	0.60	0.43	0.27	1.00	0.22
pyrene	0.51	0.06	0.36	0.46	0.32	2.01	0.14
benzo[*ghi*]fluoranthene							
cyclopenta[*cd*]pyrene	0.24		0.18				
benz[*a*]anthracene	0.13	0.64	0.08	0.45	0.11	4.54	0.26
chrysene				0.38	0.25	4.50	0.12
triphenylene							
benzo[*b*]fluoranthene	0.02	0.20	0.07	0.21	0.32	3.75	0.38
benzo[*j*]fluoranthene	0.16	0.38	0.42				
benzo[*k*]fluoranthene	0.79	0.24	0.34	0.28	0.29	5.51	0.08
benzo[*e*]pyrene	0.20	0.11	0.28	0.41	0.39	10.25	0.11
benzo[*a*]pyrene	0.49	0.97	0.13	0.60	0.08	3.44	0.64
perylene	0.56		0.40				
indeno[1,2,3-*cd*]pyrene				1.71	0.93	3.75	0.58
benzo[*ghi*]perylene	0.19	0.49	0.14	0.55	0.11	3.89	0.13
dibenz[*a,h*]anthracene				0.73	0.21	10.84	0.67
dibenz[*a,c*]anthracene	0.27		0.32				
benzo[*b*]chrysene	0.27		0.16				
coronene	0.07	0.39	0.15				
dibenzo[*a,e*]pyrene	0.19		0.27				
9-nitroanthracene							
1-nitropyrene							
2-nitrofluoranthene							
3-nitrofluoranthene							
7-nitrobenz[*a*]anthracene							
6-nitrochrysene							
6-nitrobenzo[*a*]pyrene							
9-fluoreneone							
acenaphthenequinone							
perinaphthenone							
antraquinone (9,10-AQ)							
benzanthrone							
benz[*a*]anthracene-7,12-dione							
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one							
n-C20				0.19	0.13	5.74	0.16
n-C21							
n-C22				3.11	1.46	2.30	0.18
n-C23							
n-C24				3.32	0.63	1.18	0.69
n-C25							
n-C26				1.73	0.05	1.54	0.32
n-C27							
n-C28				1.02	0.23	1.10	0.43
n-C29							
n-C30				0.36	0.46	0.77	0.22
n-C31							
n-C32				0.29	0.24	2.00	0.07
n-C40							
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)							
abb 20R 24R-Ethylcholestane (Chiron#0662,29)							
abb 20R 24S-Methylcholestane (Chiron#0643,28)							
abb 20R Cholestane (Chiron#0602,27)							
aaa 20R-Cholestane (Chiron#0622,27)							
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)							
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)							
17a(H),21b(H)-Hopane (Chiron#0132,30)							
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)							
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)							
pristane							
phytane							
cholesterol							
stigmasterol							
pimaric acid							
isopimaric acid							
pinonic acid							
hexadecanoic acid							
syringol							
isoeugenol							
levoglucosan							

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	10a				10b	
	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a	Balt-2 PM	RM 8785
naphthalene						
fluorene						
phenanthrene						
anthracene						
1-methylphenanthrene						
2-methylphenanthrene						
3-methylphenanthrene						
9-methylphenanthrene						
retene						
4H-cyclopenta[*def*]phenanthrene						
fluoranthene						
pyrene						
benzo[*ghi*]fluoranthene						
cyclopenta[*cd*]pyrene						
benz[*a*]anthracene						
chrysene						
triphenylene						
benzo[*b*]fluoranthene						
benzo[*j*]fluoranthene						
benzo[*k*]fluoranthene						
benzo[*e*]pyrene						
benzo[*a*]pyrene						
perylene						
indeno[1,2,3-*cd*]pyrene						
benzo[*ghi*]perylene						
dibenz[*a,h*]anthracene						
dibenz[*a,c*]anthracene						
benzo[*b*]chrysene						
coronene						
dibenzo[*a,e*]pyrene						
9-nitroanthracene						
1-nitropyrene						
2-nitrofluoranthene						
3-nitrofluoranthene						
7-nitrobenz[*a*]anthracene						
6-nitrochrysene						
6-nitrobenzo[*a*]pyrene						
9-fluoreneone						
acenaphthenequinone						
perinaphthenone						
antraquinone (9,10-AQ)						
benzanthrone						
benz[*a*]anthracene-7,12-dione						
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one						
n-C20	0.53					
n-C21	0.31	0.27		0.03		
n-C22	0.04	0.96	2.22	0.07		
n-C23	0.21	0.64	0.28	0.12		
n-C24	0.11	1.98	0.79	0.22		
n-C25	0.14	1.25	2.68	0.07		
n-C26	0.09	2.23	2.58	0.10		
n-C27	0.04	0.76	1.05	0.11		
n-C28	0.10	1.49	1.82	0.27		
n-C29	0.34	0.25	1.12	0.47		
n-C30	0.50	1.54	1.06	0.25		
n-C31	0.12	0.15	1.26	0.15		
n-C32	0.50	1.46	1.79	0.05		
n-C40						
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)	0.39	0.83	1.35	0.52	3.82	
abb 20R 24R-Ethylcholestane (Chiron#0662,29)	0.13	0.66	0.76	0.45	2.80	3.58
abb 20R 24S-Methylcholestane (Chiron#0643,28)	0.21			0.38	2.65	8.41
abb 20R Cholestane (Chiron#0602,27)	0.07	0.65	0.92	0.18	2.69	4.80
aaa 20R-Cholestane (Chiron#0622,27)	0.09			0.66	1.89	3.03
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	0.20	0.61	0.71	0.26	2.46	2.14
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)	0.26	0.48	1.22	0.32	2.08	1.54
17a(H),21b(H)-Hopane (Chiron#0132,30)	0.20	0.56	0.38	0.34	1.09	1.68
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	0.15	0.42	0.30	0.35	0.26	0.34
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	0.17	0.63	0.46	0.24	0.92	1.25
pristane						
phytane						
cholesterol						
stigmasterol						
pimaric acid						
isopimaric acid						
pinonic acid						
hexadecanoic acid						
syringol						
isoeugenol						
levoglucosan						

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	11				12			
	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a
naphthalene	0.23	0.71	2.67	0.50	1.72	3.50	4.80	1.75
fluorene	0.72	1.90	1.98	0.82				
phenanthrene	0.12	0.40	1.90	0.10	1.05			0.97
anthracene	0.23			0.18	1.73			0.50
1-methylphenanthrene	0.48	1.79		0.82				
2-methylphenanthrene	0.06	0.17		0.45				
3-methylphenanthrene	0.33			0.27				
9-methylphenanthrene	0.14			0.59				
retene								
4H-cyclopenta[*def*]phenanthrene								
fluoranthene	0.15	0.24	1.56	0.06	0.63	1.03	1.01	0.76
pyrene	0.11	0.26	2.05	0.06	0.94	2.13	1.57	1.02
benzo[*ghi*]fluoranthene	0.53	0.71	3.91	0.16				2.03
cyclopenta[*cd*]pyrene	0.69			1.12				1.58
benz[*a*]anthracene	0.07		2.73	0.60	0.15			0.71
chrysene	0.45	1.00	1.31	1.70	2.70			0.50
triphenylene	0.63	2.89	2.80	1.87	2.01			0.97
benzo[*b*]fluoranthene					0.82			0.31
benzo[*j*]fluoranthene					0.61			0.04
benzo[*k*]fluoranthene					0.61			0.04
benzo[*e*]pyrene	0.48	0.77	1.31	0.36	0.79			1.19
benzo[*a*]pyrene	0.48	1.20	1.04	0.32	0.35			0.78
perylene	3.25	0.96	1.71	0.56				0.00
indeno[1,2,3-*cd*]pyrene	0.74	0.29	1.03	0.21				0.71
benzo[*ghi*]perylene	0.74	0.31	0.75	0.41	0.82			1.24
dibenz[*a,h*]anthracene								
dibenz[*a,c*]anthracene								
benzo[*b*]chrysene	0.71	1.54	1.04					
coronene	0.72	1.18	0.70	0.76				3.98
dibenzo[*a,e*]pyrene	2.36		2.52	3.64				
9-nitroanthracene								
1-nitropyrene								
2-nitrofluoranthene								
3-nitrofluoranthene								
7-nitrobenz[*a*]anthracene								
6-nitrochrysene								
6-nitrobenzo[*a*]pyrene								
9-fluoreneone	0.44	0.96	2.52	0.33				
acenaphthenequinone	4.39	0.10	3.41	1.45				
perinaphthenone	0.48		1.09	0.54				
antraquinone (9,10-AQ)	0.40	1.14	1.96	0.25				
benzanthrone	0.30	0.47	1.20	4.10				
benz[*a*]anthracene-7,12-dione	0.44	0.44	0.74	0.64				
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one		1.36	1.74					
n-C20	0.44	0.81	3.47	2.53	6.38	0.98	8.23	0.45
n-C21	0.70	1.78	2.61	0.16	2.54	0.88	4.41	0.75
n-C22	0.70	1.42	2.58	0.78	6.05	1.04	8.63	1.59
n-C23	0.73	1.18	0.87	1.10	3.01	2.60	6.48	1.72
n-C24	0.76	4.59	1.91	1.27	3.61	4.55	8.13	1.73
n-C25	0.94	3.64	0.59	0.20	0.49	3.10	4.47	0.99
n-C26	0.16	3.44	2.07	0.38	1.96	4.44	6.52	0.30
n-C27	0.58	0.72	1.25	0.09	1.14	3.58	9.56	0.16
n-C28	0.27	0.49	2.50	0.76	3.84	2.10	8.07	0.20
n-C29	0.24	0.37	1.64	0.46	1.31	3.20	5.75	0.15
n-C30	0.68	0.77	4.60	0.16	5.53	4.51	8.23	0.92
n-C31	0.43	0.24	3.19	0.64	3.06	3.85	2.63	1.01
n-C32	0.77	0.87	5.05	0.98	7.12	0.00	9.64	1.46
n-C40	1.18	1.41	4.23	1.93	4.94		9.87	
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)								
abb 20R 24R-Ethylcholestane (Chiron#0662,29)								
abb 20R 24S-Methylcholestane (Chiron#0643,28)								
abb 20R Cholestane (Chiron#0602,27)								
aaa 20R-Cholestane (Chiron#0622,27)								
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)								1.47
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)								
17a(H),21b(H)-Hopane (Chiron#0132,30)					1.26		6.31	1.05
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)								
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)								
pristane							6.59	
phytane	2.86	2.84	5.56	2.14			6.48	
cholesterol		2.09	3.19		2.40	5.60	3.03	4.47
stigmasterol		0.19	2.68					
pimaric acid		2.84						
isopimaric acid	0.68	1.11	3.64	2.29				
pinonic acid					0.14		3.98	
hexadecanoic acid	0.32	1.03	2.49	0.66	1.28	3.14	6.10	
syringol				1.67				
isoeugenol	0.21							
levoglucosan	0.14	1.26	1.33	0.69	2.92	7.70	1.49	0.62

Table 7. P-scores (15%) for data reported in Trial III

Laboratory No.	13				14			
	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a	SRM 1648	Balt-2 PM	RM 8785	SRM 1649a
naphthalene					0.93	0.17	1.29	0.27
fluorene					1.23	0.83		0.63
phenanthrene					0.11	0.12	1.81	0.47
anthracene					0.06	0.20	0.91	1.23
1-methylphenanthrene								
2-methylphenanthrene								
3-methylphenanthrene								
9-methylphenanthrene								
retene								
4H-cyclopenta[*def*]phenanthrene								
fluoranthene					0.08	0.29	0.23	0.32
pyrene					0.10	0.20	0.20	0.43
benzo[*ghi*]fluoranthene								
cyclopenta[*cd*]pyrene								
benz[*a*]anthracene					0.18	0.21	0.35	0.19
chrysene					0.29	0.19	0.26	0.22
triphenylene								
benzo[*b*]fluoranthene	1.38			0.41	0.49	0.21	0.29	0.20
benzo[*j*]fluoranthene								
benzo[*k*]fluoranthene	0.88				0.76	0.81	0.63	0.44
benzo[*e*]pyrene	1.78			0.47				
benzo[*a*]pyrene					0.45	0.67	0.70	0.45
perylene								
indeno[1,2,3-*cd*]pyrene					0.41	0.58	0.23	0.56
benzo[*ghi*]perylene					0.29	0.18	0.39	0.17
dibenz[*a,h*]anthracene					0.67	1.06	0.97	0.62
dibenz[*a,c*]anthracene								
benzo[*b*]chrysene								
coronene								
dibenzo[*a,e*]pyrene								
9-nitroanthracene								
1-nitropyrene								
2-nitrofluoranthene								
3-nitrofluoranthene								
7-nitrobenz[*a*]anthracene								
6-nitrochrysene								
6-nitrobenzo[*a*]pyrene								
9-fluoreneone								
acenaphthenequinone								
perinaphthenone								
antraquinone (9,10-AQ)								
benzanthrone								
benz[*a*]anthracene-7,12-dione								
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one								
n-C20								
n-C21								
n-C22								
n-C23								
n-C24	0.68	3.50	0.72	0.63				
n-C25								
n-C26	2.34	3.09	0.96	1.90				
n-C27								
n-C28	3.26	3.32	1.47	3.72				
n-C29								
n-C30	3.00	3.60	1.17					
n-C31								
n-C32	3.48	4.20	1.44					
n-C40								
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)								
abb 20R 24R-Ethylcholestane (Chiron#0662,29)								
abb 20R 24S-Methylcholestane (Chiron#0643,28)								
abb 20R Cholestane (Chiron#0602,27)								
aaa 20R-Cholestane (Chiron#0622,27)								
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	2.23			1.18				
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)								
17a(H),21b(H)-Hopane (Chiron#0132,30)	1.25			1.19				
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	1.59			3.16				
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	1.97			2.87				
pristane								
phytane								
cholesterol								
stigmasterol								
pimaric acid								
isopimaric acid								
pinonic acid								
hexadecanoic acid								
syringol								
isoeugenol								
levoglucosan								

Table 8. Comparison of exercise assigned values for the samples in Trial III

PAHs	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
naphthalene	1038	479	46.1	2029	1997	98.4	4338	4263	98.3	1135	848	74.8	no target		Target
fluorene	242	46	19.1	227	189	83.5	2355	3120	132.5	221	52	23.7	230	50	Reference
phenanthrene	4325	1061	24.5	911	289	31.7	7600	6061	79.7	3899	709	18.2	4140	370	Certified
anthracene	463	102	21.9	118	57	48.3	1134	766	67.6	469	131	27.9	432	82	Certified
1-methylphenanthrene	424	62	14.6	156	74	47.4	808	349	43.2	363	67	18.6	370	40	Reference
2-methylphenanthrene	928	119	12.8	397	234	58.8	1243	556	44.7	766	161	21.0	730	120	Reference
3-methylphenanthrene	722	76	10.5	208	62	30.0	856	360	42.1	567	113	20.0	500	50	Reference
9-methylphenanthrene	450	76	16.9	164	97	59.1	650	288	44.3	374	41	11.0	no target		Target
retene	511	240	46.9	189	166	87.8	no assigned value			209	109	52.0	no target		Target
4H-cyclopenta[*def*]phenanthrene	284	48	16.9	107	120	112.0	no assigned value			279	57	20.4	320	60	Reference
fluoranthene	8091	849	10.5	1137	437	38.4	6057	2829	46.7	6252	614	9.8	6450	180	Certified
pyrene	6258	647	10.3	1162	294	25.3	5254	3200	60.9	5194	507	9.8	5290	250	Certified
benzo[*ghi*]fluoranthene	1135	124	10.9	225	56	25.0	1256	48	3.8	862	84	9.7	880	20	Reference
cyclopenta[*cd*]pyrene	219	43	19.4	116	18	15.4	902	59	6.6	386	234	60.7	no target		Target
benz[*a*]anthracene	2654	722	27.2	294	23	8.0	2051	798	38.9	2261	179	7.9	2210	73	Certified
chrysene	5162	1007	19.5	860	196	22.8	3874	1230	31.8	3488	1241	35.6	3049	60	Certified
triphenylene	2103	486	23.1	415	158	38.0	2118	81	3.8	1772	487	27.5	1357	54	Certified
benzo[*b*]fluoranthene	8979	1729	19.3	1334	381	28.6	8424	2202	26.1	5867	856	14.6	6450	640	Certified
benzo[*j*]fluoranthene	3237	351	10.8	755	473	62.6	2461	416	16.9	1627	376	23.1	1500	400	Reference
benzo[*k*]fluoranthene	3228	336	10.4	424	48	11.4	2470	742	30.0	2217	975	44.0	1913	31	Certified
benzo[*e*]pyrene	4913	1368	27.8	881	236	26.8	4452	365	8.2	3362	455	13.5	3090	190	Certified
benzo[*a*]pyrene	2601	335	12.9	421	126	30.0	2395	619	25.9	2419	236	9.8	2509	87	Certified
perylene	682	86	12.6	198	156	78.8	748	619	82.7	646	42	6.5	646	75	Certified
indeno[1,2,3-*cd*]pyrene	4187	801	19.1	716	115	16.1	4737	1279	27.0	3022	498	16.5	3180	720	Certified
benzo[*ghi*]perylene	5106	555	10.9	1175	440	37.4	6969	1834	26.3	4102	580	14.1	4010	910	Certified
dibenz[*a,h*]anthracene	467	100	21.4	67.7	15.2	22.5	738	803	108.7	332	141	42.4	288	23	Certified
dibenz[*a,c*]anthracene	450	65	14.5	98.2	5.8	5.9	no assigned value			296	89	30.0	200	25	Certified
benzo[*b*]chrysene	386	61	15.7	56.6	3.6	6.4	no assigned value			341	60	17.7	315	13	Certified
coronene	2632	306	11.6	587	142	24.1	10358	5321	51.4	3486	383	11.0	no target		Target
dibenzo[*a,e*]pyrene	640	92	14.3	170	9	5.6	no assigned value			593	144	24.2	630	80	Reference

Table 8. continued

nitro-PAHs	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
9-nitroanthracene	168	1	0.8	82	2	2.7	46.6	3.7	8.0	35.8	4.8	13.3	33.4	6.1	Target
1-nitropyrene	80.3	16.5	20.6	32.4	5.2	16.2	189	137	72.3	65.0	3.1	4.8	70.9	4.3	Target
2-nitrofluoranthene	297	64	21.5	316	5	1.5	717	453	63.2	310	9	2.8	313	38	Target
3-nitrofluoranthene	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
7-nitrobenz[*a*]anthracene	83.6	7.4	8.9	No assigned value			63.4	17.7	27.9	26.1	3.2	12.4	27.8	6.7	Target
6-nitrochrysene	No assigned value			No assigned value			No assigned value			No assigned value			4.01	0.52	Target
6-nitrobenzo[*a*]pyrene	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target

PAH-Quinone	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
1,2-naphthoquinone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
1,4-naphthoquinone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
9-fluoreneone	998	241	24.2	363	96	26.4	No assigned value			1140	63	5.5	no target		Target
acenaphthenequinone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
perinaphthenone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
antraquinone (9,10-AQ)	3607	697	19.3	658	399	60.6	No assigned value			2787	296	10.6	no target		Target
benzanthrone	1024	1091	106.6	682	486	71.2	No assigned value			782	297	38.0	no target		Target
benz[*a*]anthracene-7,12-dione	3121	1225	39.2	1015	342	33.6	No assigned value			2833	1433	50.6	no target		Target
1,4-chrysenequinone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target

Table 8. continued

Alkanes and alkenes	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
n-C20	2474	1283	51.8	3025	1628	53.8	49598	32176	64.9	2286	689	30.2	no target		Target
n-C21	3406	1915	56.2	3488	3655	104.8	19458	446	2.3	2909	1275	43.8	no target		Target
n-C22	6898	3268	47.4	2316	821	35.4	103849	99679	96.0	4934	1338	27.1	no target		Target
n-C23	8400	2065	24.6	5387	2060	38.2	35999	21399	59.4	14377	2814	19.6	no target		Target
n-C24	18762	7130	38.0	3575	1672	46.8	84067	70739	84.1	21529	8187	38.0	no target		Target
n-C25	59986	28043	46.7	10240	5005	48.9	133314	101428	76.1	78502	15487	19.7	no target		Target
n-C26	49986	17838	35.7	9465	4967	52.5	131565	96266	73.2	62722	28041	44.7	no target		Target
n-C27	46332	17656	38.1	23370	9629	41.2	347984	432878	124.4	72001	15381	21.4	no target		Target
n-C28	24762	9224	37.3	11930	4139	34.7	79345	56505	71.2	31371	15412	49.1	no target		Target
n-C29	45541	12885	28.3	39039	16028	41.1	131999	78746	59.7	66737	16614	24.9	no target		Target
n-C30	14102	6320	44.8	9187	3486	37.9	66977	38732	57.8	17351	7020	40.5	no target		Target
n-C31	33870	15345	45.3	32007	16344	51.1	69239	70863	102.3	38398	9300	24.2	no target		Target
n-C32	9669	3855	39.9	9625	5650	58.7	54312	39255	72.3	10964	2992	27.3	no target		Target
n-C40	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
n-C44	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
squalene	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
1-octadecene	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target

Hopanes, Cholestanes, Sterols	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
abb 20R 24R-Ethylcholestane (Chiron#0662,29)	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
abb 20R 24S-Methylcholestane (Chiron#0643,28)	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
abb 20R Cholestane (Chiron#0602,27)	1413	100	7.1	No assigned value			No assigned value			1400	1084	77.4	no target		Target
aaa 20R-Cholestane (Chiron#0622,27)	830	32	3.9	249	166	66.7	No assigned value			1344	251	18.7	no target		Target
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)	1692	55	3.3	193	43	22.4	No assigned value			4377	3373	77.1	no target		Target
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)	No assigned value			747	57	7.6	No assigned value			No assigned value			no target		Target
17a(H),21b(H)-Hopane (Chiron#0132,30)	17037	10059	59.0	No assigned value			33871	14165	41.8	26809	18426	68.7	no target		Target
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)	4018	1578	39.3	No assigned value			No assigned value			6339	417	6.6	no target		Target
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)	3653	349	9.6	No assigned value			No assigned value			5191	411	7.9	no target		Target
pristane	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
phytane	626	210	33.5	1252	250	20.0	50983	28435	55.8	979	729	74.4	no target		Target
cholesterol	4146	4123	99.5	16213	19514	120.4	124752	105172	84.3	15900	19709	124.0	no target		Target
stigmasterol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target

Table 8. continued

Carbonyls and Acids	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
G-nonanoic lactone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
G-decanolactone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
9-anthraldehyde	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
syringaldehyde	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
pimaric acid	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
isopimaric acid	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
pinic acid	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
pinonic acid	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
hexadecanoic acid	216742	112210	51.8	145987	81945	56.1	2855937	2308061	80.8	500336	142463	28.5	no target		Target
norpinic acid	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
norpinonic acid	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
nopinone	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
pinionaldehyde	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
caronaldehyde	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target

Phenols	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
syringol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
4-ethylsyringol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
isoeugenol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
propionylsyringol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
butyrylsyringol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
guaiacol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
4-methylguaiacol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target
4-ethylguaiacol	No assigned value			No assigned value			No assigned value			No assigned value			no target		Target

Sugars	SRM 1648 Exercise Assigned			Baltimore-2 PM Exercise Assigned			RM 8785 Exercise Assigned			SRM 1649a Exercise Assigned			From 1649a Certif.		
	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	Assigned	s	%RSD	conc.	95%CL	type
levoglucosan	101947	68612	67.3	106176	86131	81.1	206751	85270	41.2	46276	28977	62.6	no target		Target

Table 9. Summary of z and p scores by laboratory for each material

	total reported	absolute value of z scores (25%)				absolute value of z scores (s)				absolute value of p scores (15%)			
		0 to 1	1 to 2	2 to 3	>3	0 to 1	1 to 2	2 to 3	>3	0 to 1	1 to 2	2 to 3	>3
Lab 1a													
SRM 1648	49	45	3			47	1			48	1		
Baltimore-2 PM	45	33	9	3		42	3			45			
RM 8785	26	10	10	2	1	22	1			26			
SRM 1649a	49									49			
Lab 1b													
SRM 1648	29	27	2			27	2			29			
Baltimore-2 PM	28	19	8	1		25	3			28			
RM 8785	20	15	5			19	1			11	6	2	1
SRM 1649a	29									29			
Lab 1c													
SRM 1648	35	26	6	1		27	6			34		1	
Baltimore-2 PM	35	25	5	1	2	30	2	1		34	1		
RM 8785	26	14	2	4	2	17	4		1	9	15	2	
SRM 1649a	28									15	3		
Lab 2													
SRM 1648	15	15				14	1			13	2		
Baltimore-2 PM	15	8	7			10	5			14			1
RM 8785	14		6	3	4	4	7	1	1		10	2	2
SRM 1649a	15									15			
Lab 3a													
RM 8785	14	7	3	4		14					9	3	2
SRM 1649a	14										10	4	
Lab 3b													
RM 8785	18	8	7	3	1	13	4	2			15	2	1
SRM 1649a	19									18	1		
Lab 4													
RM 8785	34	12	3	3	14	21	10		1		4	12	18
SRM 1649a	35									24	4	3	4
Lab 5													
SRM 1648	20	12	5	3		19	1			17	3		
Baltimore-2 PM	20	3	6	8	3	9	11			9	8	1	2
SRM 1649a	20									16	3	1	
Lab 6													
SRM 1648	17	9	2		6	7	4	1	5	12	4	1	
Baltimore-2 PM	12	6	4	2		6	6			6	3		3
SRM 1649a	17									10	4	2	1
Lab 7													
SRM 1648	26	19	2		2	15	6		2	26			
Baltimore-2 PM	21	13	3	1	2	17	1		1	21			
RM 8785	18	9	5	1	3	12	5		1	6	6	4	2
SRM 1649a	26									26			
Lab 8													
SRM 1648	25	21	2	2		7	18			25			
Baltimore-2 PM	20	3	4	3	10	3	13	2	2	19	1		
SRM 1649a	25									25			
Lab 9													
SRM 1648	25	13	9	1	1	14	7	1	2	16	4	3	2
Baltimore-2 PM	25	12	6	2	5	16	7	1	1	23	2		
RM 8785	24	6	6	9	3	17	5		2	2	6	3	13
SRM 1649a	25									25			

Table 9 cont. Summary of z and p scores by laboratory for each material

Lab 10a													
SRM 1648	23	9	8	2		12	7			23			
Baltimore-2 PM	20	7	5	2		12	2			14	5	1	
RM 8785	19	5	7	3		14	1			8	8	3	
SRM 1649a	22									22			
Lab 10b													
Baltimore-2 PM	10	2	1			2	1			2	2	5	1
RM 8785	9	1				1	1			1	3	1	4
Lab 11													
SRM 1648	48	20	11	3	10	23	13	1	7	43	1	2	2
Baltimore-2 PM	44	11	12	5	11	16	14		9	23	14	4	3
RM 8785	44	1	5	6	21	11	6	2	14	6	17	12	9
SRM 1649a	47									34	8	3	2
Lab 12													
SRM 1648	33	7	6	11	6	8	16	1	5	11	8	5	9
Baltimore-2 PM	21	9	7	4	1	14	6		1	5	2	3	11
RM 8785	24	4	3	6	9	11	10		1		3	1	20
SRM 1649a	36									21	12	1	2
Lab 13													
SRM 1648	12	3	5	3	1	6	5		1	2	5	3	2
Baltimore-2 PM	5	2	3			5							5
RM 8785	5	2	2	1		5				2	3		
SRM 1649a	9									3	3	1	2
Lab 14													
SRM 1648	14	12	1	1		8	6			13	1		
Baltimore-2 PM	14	11	2	1		14				13	1		
RM 8785	13	6	7			6	7			11	2		
SRM 1649a	14									13	1		

Intercomparison Exercise: Trial III
Description of Materials and Instructions

Intercomparison Exercise Materials (none of the following have been enriched or spiked):

Trial IIIa –

SRM 1648 (St. Louis PM)

Each bottle contains approximately 500 mg of SRM 1648. This material was collected in a baghouse over a 12+ month period in the mid 1970s. The bottled material passed through a 53 μm sieve and was blended.

Baltimore #2 PM2.5

Each bottle contains approximately 100 mg of a PM collected from the same site as the material used in Trial II but during the fall of 2002. The particle size of the material is nominally 2.5 μm and less.

Trial IIIb –

RM 8785 (Air Particulate Matter on Filter Media)

Each participant receives four quartz-fiber filters with a fine fraction of SRM 1649a, Urban Dust, suspended on them. The mass of PM on each filter is noted on the holder.

Control Material for Trial III –

SRM 1649a

Each bottle contains approximately 500 mg of SRM 1649a.

Instructions for Use:

Please analyze three samples each of SRM 1648, Baltimore #2, and SRM 1649a and/or the four filters (depending on the samples requested), using **your** laboratory's and/or program's analytical protocols, for the concentrations (mass/mass) of the analytes listed in Table 1. If your laboratory is not measuring some of these target compounds, then you do not need to report values for those analytes in this exercise. There is space provided at the bottom of the spreadsheet to report additional analytes of interest to your program. Please provide data for all of the compounds that your laboratory is quantifying in the PM 2.5 program. All data received will be summarized.

Reporting of Results:

Please report one result, as if three figures were significant, for each of the analytes in each of the samples analyzed. Report results in units of ng/g as received for the air particulate samples and filters. Be sure to keep the bottles well sealed and bring to room temperature before weighing if stored in the refrigerator or freezer. Report the date of measurement of each sample in the requested m/d/y format.

We recognize that the reported concentrations for some of the requested analytes will probably include concentrations of compounds reported to coelute with the analyte of interest with methods commonly in use. Please note at the bottom of your table of reported results if any coelution qualifiers are applicable to your data. Please note that any changes that you make to the column or row headings **within** the tables will **not** be seen by the coordinators because only the table entries and comments at the bottom of the tables are automatically transferred to the exercise database. Please do not add or delete lines from the spreadsheet.

We prefer that concentration values be reported for each analyte determined. If the measured concentration is below your typical reporting concentration for an analyte in a particular matrix, you can report the number and list the appropriate detection limit, quantification limit, etc. at the bottom of the data table. However, if you need to report non-numerical data please use the following conventions:

NA	"Not analyzed", "not determined"
<"value"	"Less than specified concentration", e.g., <8 ng/g
Other	"Other"; add note of explanation at end of data table, e.g., interference
DL	"Below detection limit" may be used, however, <"value" is preferable

Do not use negative numbers or parentheses to indicate "less than detection limits".

An EXCEL file, APT03.xls, has been sent as an e-mail attachment to you. If you have any software/hardware conversion problems, please contact Michele Schantz. The data file templates also include places for you to list the surrogate/internal standards and type of calibration curve used, and to provide a brief description of the analyses. Please **do not** add spaces before entering numbers in the table cells and enter them as "numbers" not as "labels". Please **do not** insert any columns or rows **within** the table in the data file. If you wish to include additional data and/or other information or comments, you may add it to the bottom of the data table in the diskette file or send it in hard copy. A printout of the data file format is shown in Table 1.

Submit your results as an attached file via e-mail (preferred) to:

E-mail: michele.schantz@nist.gov

The deadline for receipt of data is January 15, 2005.

Further Information:

If you need further information, please contact Michele at the e-mail listed above or at the following phone numbers: Phone: (301)975-3106
FAX: (301)977-0685

Table 1. Diskette Data File Format (File: APT03.*)

Intercomparison Exercise Program for Organics in PM 2.5 Air Particulate Matter
Trial III

Please fill in all blanks; Use requested units of concentration; Report results as if 3 figures were significant
DO NOT INSERT ROWS OR COLUMNS WITHIN THIS TABLE. DO NOT MOVE CELLS.
- If necessary, add additional data/information at the end of the table.
- Use one of the following if no concentration is reported for an analyte:
  NA = Not analyzed/determined; <"conc" = <detection limit conc.; Other = other, explain in a note at end of table
  (DL = "below detection limit" may be used, but <"conc", e.g., <8, is preferable.)
  Do not use parentheses or negative numbers to indicate "less than detection limit".

Reporting Date (m/d/y): _____
Laboratory: _____
Submitted by: _____

BRIEF DESCRIPTION OF PROCEDURES USED:

Approximate amount of sample extracted:

SRM 1648 _____ g, as received
Baltimore 2 PM _____ g, as received
Filter 1 _____ µg, as received
Filter 3 _____ µg, as received
SRM 1649a _____ g, as received
Filter 2 _____ µg, as received
Filter 4 _____ µg, as received

Extraction method: _____
Extraction solvent: _____
Extraction time: _____
Extraction - other: _____

Sample extract cleanup method: _____

Analytical method used (e.g., GC-FID, GC-ECD):

	Analyt. Instr.	Column Phase	Col. Length, m	Col. i.d., mm	Col. film thickness, µm
PAH					
Nitro PAH					
PAH-quinone					
Alkanes and Alkenes					
Hopanes, Cholestanes, Sterols					
Carbonyls and Acids					
Phenols					
Sugars					

Method of quantitation (IS = internal standard, ES = external standard):

PAHs _____
Nitro-PAHs _____
PAH-quinone _____
Alkanes and Alkenes _____
Hopanes, Cholestanes, Sterols _____
Carbonyls and Acids _____
Phenols _____
Sugars _____

IF internal standard method was used, please complete the following section:
Identity of internal standards/surrogates used that were:
Added PRIOR to extraction of sample:

PAHs _____
Nitro-PAHs _____
PAH-quinone _____
Alkanes and Alkenes _____
Hopanes, Cholestanes, Sterols _____
Carbonyls and Acids _____
Phenols _____
Sugars _____

Added after extraction/cleanup and JUST PRIOR to chromatographic analysis:

PAHs _____
Nitro-PAHs _____
PAH-quinone _____
Alkanes and Alkenes _____
Hopanes, Cholestanes, Sterols _____
Carbonyls and Acids _____
Phenols _____
Sugars _____

Any others? Added at what point in analyses: _____

PAHs _____
Nitro-PAHs _____
PAH-quinone _____
Alkanes and Alkenes _____
Hopanes, Cholestanes, Sterols _____
Carbonyls and Acids _____
Phenols _____
Sugars _____

IS/surrogate standards used for quantitation calculations were:
_____ those added prior to extraction
_____ those added after extraction/cleanup and just prior to chromatographic analysis
If the IS/surrogates added after extraction/cleanup extraction were used for quantitation, were results corrected for percent recovery? _____
Percent recovery range:

PAHs _____
Nitro-PAHs _____
PAH-quinone
Alkanes and Alkenes _____
Hopanes, Cholestanes, Sterols _____
Carbonyls and Acids _____
Phenols _____
Sugars _____

Calibration Curve

	Points	Conc. Range	Analytes outside of calibration curve calibration range
PAH			
Nitro PAH			
PAH-quinone			
Alkanes and Alkenes			
Hopanes, Cholestanes, Sterols			
Carbonyls and Acids			
Phenols			
Sugars			

Please note any differences in procedures used for SRM 1649a analyses from those described above:

_____

RESULTS:

PAH ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
naphthalene														
fluorene														
phenanthrene														
anthracene														
1-methylphenanthrene														
2-methylphenanthrene														
3-methylphenanthrene														
9-methylphenanthrene														
retene														
4H-cyclopenta[*def*]phenanthrene														
fluoranthene														
pyrene														
benzo[*ghi*]fluoranthene														
cyclopenta[*cd*]pyrene														
benz[*a*]anthracene														
chrysene														
triphenylene														
benzo[*b*]fluoranthene														
benzo[*j*]fluoranthene														
benzo[*k*]fluoranthene														
benzo[*e*]pyrene														
benzo[*a*]pyrene														
perylene														
indeno[1,2,3-*cd*]pyrene														
benzo[*ghi*]perylene														
dibenz[*a,h*]anthracene														
dibenz[*a,c*]anthracene														
benzo[*b*]chrysene														
coronene														
dibenzo[*a,e*]pyrene														

Nitro-PAH ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
9-nitroanthracene														
1-nitropyrene														
2-nitrofluoranthene														
3-nitrofluoranthene														
7-nitrobenz[*a*]anthracene														
6-nitrochrysene														
6-nitrobenzo[*a*]pyrene														

PAH-Quinone ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
1,2-naphthoquinone														
1,4-naphthoquinone														
9-fluoreneone														
acenaphthenequinone														
perinaphthenone														
antraquinone (9,10-AQ)														
benzanthrone														
benz[*a*]anthracene-7,12-dione														
1,4-chrysenequinone														
9,10-dihydrobenzo[*a*]pyrene-7(8H)-one														
Alkanes and Alkenes	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
n-C20														
n-C21														
n-C22														
n-C23														
n-C24														
n-C25														
n-C26														
n-C27														
n-C28														
n-C29														
n-C30														
n-C31														
n-C32														
n-C40														
n-C44														
squalene														
1-octadecene														

Hopanes, Cholestanes, Sterols	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
aaa 20R 24R-Ethylcholestane (Chiron#0609,29)														
abb 20R 24R-Ethylcholestane (Chiron#0662,29)														
abb 20R 24S-Methylcholestane (Chiron#0643,28)														
abb 20R Cholestane (Chiron#0602,27)														
aaa 20R-Cholestane (Chiron#0622,27)														
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)														
17a(H),21b(H)-30-Norhopane (Chiron#1321,29)														
17a(H),21b(H)-Hopane (Chiron#0132,30)														
17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)														
17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)														
pristane														
phytane														
cholesterol														
stigmasterol														

Carbonyls and Acids	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
G-nonanoic lactone														
G-decanolactone														
9-anthraldehyde														
syringaldehyde														
pimaric acid														
isopimaric acid														
pinic acid														
pinonic acid														
hexadecanoic acid														
norpinic acid														
norpinonic acid														
nopinone														
pinlonaldehyde														
caronaldehyde														

Phenols	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1 (ng/g as received)	SRM 1648 Sample 2 (ng/g as received)	SRM 1648 Sample 3 (ng/g as received)	Baltimore 2 PM Sample 1 (ng/g as received)	Baltimore 2 PM Sample 2 (ng/g as received)	Baltimore 2 PM Sample 3 (ng/g as received)	Filter 1 (ng/g as received)	Filter 2 (ng/g as received)	Filter 3 (ng/g as received)	Filter 4 (ng/g as received)	Filter Blank (ng/g as received)	SRM 1649a Sample 1 (ng/g as received)	SRM 1649a Sample 2 (ng/g as received)	SRM 1649a Sample 3 (ng/g as received)
syringol														
4-ethylsyringol														
isoeugenol														
propionylsyringol														
butyrylsyringol														
guaiacol														
4-methylguaiacol														
4-ethylguaiacol														
Sugars	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a	SRM 1649a	SRM 1649a
Analyst (Initials)														
Date(s) of measurements (m/d/y)														
	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
levoglucosan														

Any additional data/information should be added here.

Appendix B

Laboratory Notes Accompanying Data

Lab	Additional notes for Submitted with the Trial III data
1b	filter blank values reported in ng filter analytes are blank substracted one additional sample of SRM 1648 reported at right one additional sample of Baltimore 2 PM reported at right chrysene and triphenylene separated on liquid cyrstal column

additional analytes:

PAH ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
	(ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as receiv	ng	g/g as receiv	g/g as receiv	(ng/g as received)
1,2-DIMETHYLNAPHTHALENE	<150	<150	<150	<62	<62	<62	<1700	<1700	<1700	<1700	1.18	<150	<150	<150
2-METHYLANTHRACENE	<130	<130	<130	<33	<33	<33	<230	<230	<230	<230	0.143	<140	<140	<140
1,7-dimethylphenanthrene	281	275	290	98.1	96.9	101	<670	<670	<670	<670	DL	249	258	258
3-METHYLFLUORATHENE	456	468	480	70.1	68	71.8	<440	<440	<440	<440	DL	323	335	369
1-METHYLFLUORANTHENE	205	202	211	27.3	31.1	28.8	<250	<250	<250	<250	DL	146	146	165
4-METHYLPYRENE	399	392	409	74.6	80.5	75.2	<500	<500	<500	<500	DL	297	305	325
1-METHYLPYRENE	281	292	299	55.3	55	55.2	<490	<490	<490	<490	DL	218	222	251
3-METHYLCHRYSENE	341	334	376	50.9	53.5	58.4	<450	<450	<450	<450	DL	241	224	250
6-METHYLCHRYSENE	209	215	210	40.5	43.6	37.7	<610	<610	<610	<610	DL	177	171	165
4-METHYLPHENANTHRENE	<35	<35	<35	<10	<10	<10	NA	NA	NA	NA	NA	30	23	24
8-methylfluoranthene	273	275	281	38.4	43.1	40.1	NA	NA	NA	NA	NA	225	230	248
2-methylpyrene	487	497	510	104	108	105	NA	NA	NA	NA	NA	408	420	466
biphenyl	549	283	496	160	157	216	<5600	<5600	<5600	<5600	3.70	388	342	330
acenaphthylene	98	89	103	47.1	48.4	47.5	<940	<940	<940	<940	0.313	<140	<140	<140
dibenzothiophene	305	293	293	46	45.8	46.5	<330	<330	<330	<330	0.202	234	206	236
benzo[*c*]phenanthrene	867	843	887	96.5	102	98.2	<700	<700	<700	<700	DL	464	475	493
benzo[*a*]fluoranthene	460	472	474	72	72.8	85.2	<500	<500	<500	<500	DL	436	471	496
dibenz[*a,j*]anthracene	491	466	482	88.8	91.2	94.7	DL	DL	DL	DL	DL	343	339	347
picene	730	721	803	131	131	133	DL	DL	DL	DL	DL	459	468	496
anthanthrene	699	713	741	136	150	150	1185	915	924	981	DL	734	775	793
dibenzo[*b,k*]fluoranthene	997	983	1025	<160	<160	<160	DL	DL	DL	DL	DL	649	744	758
dibenzo[*a,h*]pyrene	<220	<220	<220	DL	DL	DL	DL	DL	DL	DL	DL	<240	<240	<240
chrysene and triphenylene (in combination DB17)	8313	8317	8429	1363	1388	1390	6264	5384	6457	5835	DL	4659	4652	4861

4-METHYLPHENANTHRENE quantified using 1-methylphenanthrene
8-methylfluoranthene quantified using 3-methylfluoranthene
2-methylpyrene quantified using 4-methylpyrene

Lab	Additional notes for Submitted with the Trial III data
3b	The concentration of chrycene includes also triphenylene. other = Naphthalene could not be quantified because the filters 2 and 3 evaporated to dryness, accidently.

additional analytes:

PAH ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
	(ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as receiv	g/g as receiv	g/g as receiv	g/g as receiv	(ng/g as received)
1,7-dimethylphenanhtrene							385	567	433	763	0.4	213	188	186

Lab	Additional notes for Submitted with the Trial III data
4	Actually the chrysene value is the sum of chrysene plus triphenylene Blank values are given in ng instead of ng/g

#	Additional Compounds	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
5		(ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as receive	(ng/g as received)
	Heptadecanoic acid	12764	13469	11255	6753	7326	7163						25686	25675	24505
	Octadecanoic acid	252968	222194	242737	60098	69024	72256						188595	188308	188595
	Eicosanoic acid	11387	11646	14376	25533	29956	27990						25181	27933	23055
	Heneicosanoic acid	19501	21136	24196	5300	6172	4917						43065	41348	42778
	Docosanoic acid	14087	11760	13046	13042	19694	16610						20293	21323	12714
	Tricosanoic acid	16341	12010	13935	15069	18345	17408						24442	24225	23445
	Tetracosanoic acid	38012	36631	36677	27135	45584	40405						48069	46926	42514
	1-tetracosanol	8535	8042	9003	12955	15246	13439						11549	12014	12943
	1-hexacosanol	21276	21864	18916	22118	25882	22773						27318	30616	25758
	1-octacosanol	31984	35328	31510	25050	28810	29020						30983	30862	30918
	2-Tetradecanone	2547	3522	2772	3178	6805	4519						8003	4789	7116
	2-Pentadecanone	2057	2216	2016	2183	1368	2767						3391	3697	3462
	2-Hexadecanone	1982	1950	2113	2692	2853	2837						2854	3051	2957
	2-Heptadecanone	2326	1989	1619	2907	7829	2840						4034	3544	3798
	2-Octadecanone	2068	1784	1238	721	2655	2264						2413	3189	2364
	2-Nonadecanone	1435	1407	1399	1142	1633	1785						2582	1820	2419

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1. The methylphenanthrenes were analyzed, however, the values obtained were overestimated from 2 to 4 times with our analytical method.

2. The sum chrysene+triphenylene, benzo(b+j+k)fluoranthenes and dibenz[a,c+a,h]anthracene was determined for all samples

	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
	(ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as receive	(ng/g as received)
chrysene+triphenylene	6269	11248	10437	733	377	Other						3859	7197	6583
benzo(b+j+k)fluoranthenes	24326	27952	21492	1885	2066	Other						14541	15476	14518
dibenz[a,c+a,h]anthracene	584	572	495	< 315	< 315	Other						518	306	358

3. For Baltimore 2 PM, the analysis was made by duplicate

#	ADDITIONAL PAH ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
7		(ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as receive	(ng/g as received)
	Acenapthylene	45.2	57	48.9	43.9	30.9	49.1	1100	500	1100	500	1.4	57.8	59.5	75.7
	Acenaphthene	145.6	132.5	160.1	103.1	108.4	102.6	2800	1500	3700	1200	4	126.6	127.7	177.7
	2-Methylfluorene	86.5	79.6	96.4	191	160.3	192.9	4800	2800	6300	2200	6.4	99.9	108	119.8
	Benzo(a)fluorene	347.8	315.2	345.9	102.5	93	108.5	1500	1200	1900	900	1.6	303.9	325.4	377.5
	Benzo(b)fluorene	117	109.3	121.4	55.2	49.5	59.4	1100	800	1500	600	1.2	113.5	125.3	143.7
	1-Methylpyrene	342.4	312.7	345.7	77.4	75	89.8	1400	900	1900	800	1.4	246.7	238.8	270.8
	7-Methylbenz(a)anthracene	16.7	14.7	15.2	<33.1	<33.3	<33.3	<1100	<800	<1500	<600	<1.0	12.1	12	13.5
	3-Methylcholanthrene	<69.6	<69.8	<69.7	<231.8	<233.3	<233.3	<7600	<5900	<10600	<4200	<7.0	<69.7	<69.6	<69.9
	Indeo(123)fluoranthene	328.7	304.9	330	<99.3	<100.0	<100.0	<3300	<2500	<4600	<1800	<3.0	204.6	223.2	243.2
	Anthanthrene	344.1	320.5	358.1	<331.1	<333.3	<333.3	<10900	<8500	<15200	<6000	<10.0	323.7	360.3	384

7 cont	NOTE:	1. benzo(j)fluoranthene and benzo(k)fluoranthene are coeluted, so the value for these two compounds are same 2. Surrogates added to samples PRIOR to extraction of sample for PAH analysis are: d10-Naphthalene d10-Acenapthylene d10-Acenapthene d10-Fluorene d10-Phenanthrene d10-Anthracene d10-Pyrene d12-Benzo(a)anthracene d12-Triphenylene d12-Chrysene d12-Benzo(b)fluoranthene d12-Benzo(e)pyrene d12-Benzo(a)pyrene d12-Perlene d12-Indeno(123-cd)pyrene d14-Dibenzo(ah)anthracene d12-Benzo(ghi)perylene 3. There is no filter blank sample for PAH and Nitro-PAH analysis, instead of that there is the method blank sample consisting of Acetone/Hexanes, results unit is ng, not ng/g 4. Surrogates added to samples PRIOR to extraction of sample for nPAH analysis are: 2-nilrofluorene-d9 9-nilroanthracene-d9 3-nilrofluoranthene-d9 1-nilropyrene-d9 6-nilrochrysene-d11 6-nilrobenzo(a)pyrene-d11 1,3-dinilropyrene-d8 1,6-dinilropyrene-d8 1,8-dinitropyrene-d8 1-nilrobenzo(e)pyrene-d11 3-nilrobenzo(e)pyrene-d11

9	ADDITIONAL PAH ANALYSES	SRM 1648 Sample 1	SRM 1648 Sample 2	SRM 1648 Sample 3	Baltimore 2 PM Sample 1	Baltimore 2 PM Sample 2	Baltimore 2 PM Sample 3	Filter 1	Filter 2	Filter 3	Filter 4	Filter Blank	SRM 1649a Sample 1	SRM 1649a Sample 2	SRM 1649a Sample 3
		(ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ng/g as received	ɔ/g as receiv	ɔ/g as receiv	ɔ/g as receiv	ɔ/g as receiv	(ng/g as received)
	2-Methylanthracene	166	198	222	172	179	176	1358	817	1073	1867	DL	172	177	176
	1,7-Dimethylphenanthrene	87	126	75.5	DL	DL	DL	1185	404	DL	DL	DL	73.6	95.7	98.4
	1-Methylfluoranthene	274	294	300	336	347	334	217	162	203	DL	DL	286	279	292
	3-Methylfluoranthene	211	265	210	55.7	47.8	48.7	648	212	294	446	173	173	176	154
	4-Methylpyrene	223	243	298	142	154	151	1427	575	881	1572	979	210	204	213
	1-Methylpyrene	314	347	363	418	415	408	3538	1842	2587	4406	2955	311	307	314
	3-Methylchrysene	682	835	984	263	296	299	1683	1288	1614	2151	DL	403	427	517
	6-Methylchrysene	573	659	734	106	100	97.2	1303	938	1191	954	91.4	931	776	714

10a

1 For Alkanes < C26, LOD is 0.15ug/ml; >C26 LOD is 0.30ug/ml extract
2 Prystane and Phytane, LOD is 0.15ug/ml extract
3 Hopanes and steranes: LOD is 0.02ug/ml extract
4 alkylcyclohexanes: LOQ = 0.15ug/ml extract
5 samples SRM1649 were concentrated to 0.2 ml prior to analysis; all other samples were concentrated to 0.10 ml prior to analysis
6 Alkylcyclohexanes were also analyzed

Calibration Cur	Points	Conc. Range	
	3	0.2, 0.5, 1.0 µg/mL	for the PM
	3	0.05, 0.10 and 0.50 µg/mL	for the filters.

6. Alkylcyclohexane Analysis	SRM 1648 Sample 1 (ng/g as received	SRM 1648 Sample 2 ng/g as received	SRM 1648 Sample 3 ng/g as received	Baltimore 2 PM Sample 1 ng/g as received	Baltimore 2 PM Sample 2 ng/g as received	Baltimore 2 PM Sample 3 ng/g as received	Filter APM0581 ng/g as received	Filter APM1505 ng/g as received	Filter APM2271 ng/g as received	Iter APM11: ng/g as received	Blank APM ng/g as receiva	SRM 1649a Sample 1 g as receiv	SRM 1649a Sample 2 g as receiv	SRM 1649a Sample 3 (ng/g as received)
1) n-Dodecylcyclohexane	<400	<400	<400	<400	<400	<400	<3000	<3000	<3000	<3000	<15	<400	<400	<400
2) n-Tridecylcyclohexane	<400	<400	<400	<400	<400	<400	<3000	<3000	<3000	<3000	<15	<400	<400	<400
3) n-Tetradecyl-cyclohexane	<400	<400	<400	<400	<400	<400	<3000	<3000	<3000	<3000	<15	<400	<400	<400
4) n-Pentadecyl-cyclohexane	<400	<400	<400	<400	<400	<400	<3000	<3000	<3000	<3000	<15	<400	<400	<400
5) n-Hexadecyl-cyclohexane	<400	<400	<400	<400	<400	<400	<3000	<3000	<3000	<3000	<15	<400	<400	<400
6) n-Heptadecyl-cyclohexane	1137	912	1102	<400	<400	<400	<9000	<9000	<9000	<9000	<15	908	944	1095
7) n-Octadecyl-cyclohexane	988	730	939	<400	<400	<400	<9000	<9000	<9000	<9000	<15	1234	1271	1475
8) n-Nonadecyl-cyclohexane	1285	958	1266	<400	<400	<400	<9000	<9000	<9000	<9000	<15	1525	1598	1812
9) n-Eicosyl-cyclohexane	1433	1186	1388	<400	<400	<400	<9000	<9000	<9000	<9000	<15	1271	1271	1496

11 Analyses are color coded by GC/MS method (3: alkanes, PAH, and POC)

Additional alkanes (in chromatographic elution order)

	SRM 1648 Sample 1 (ng/g as received	SRM 1648 Sample 2 ng/g as received	SRM 1648 Sample 3 ng/g as received	Baltimore 2 PM Sample 1 ng/g as received	Baltimore 2 PM Sample 2 ng/g as received	Baltimore 2 PM Sample 3 ng/g as received	Filter APM0581 ng/g as received	Filter APM1505 ng/g as received	Filter APM2271 ng/g as received	Iter APM11: ng/g as received	Blank APM ng/g as receiva	SRM 1649a Sample 1 g as receiv	SRM 1649a Sample 2 g as receiv	SRM 1649a Sample 3 (ng/g as received)
undecane	3.52E+03	3.76E+03	3.47E+03	1.17E+04	1.20E+04	1.25E+04	4.53E+05	2.66E+05	3.73E+05	7.97E+05	0.585	2.02E+03	2.08E+03	2.38E+03
dodecane	2.05E+03	1.98E+03	1.71E+03	5.86E+03	6.97E+03	7.61E+03	3.68E+05	1.94E+05	2.89E+05	5.23E+05	0.567	9.06E+02	1.05E+03	7.54E+02
tridecane	2.64E+03	2.45E+03	2.44E+03	7.06E+03	7.85E+03	6.19E+03	3.24E+05	2.57E+05	2.08E+05	6.78E+05	0.542	3.16E+03	2.84E+03	4.68E+03
norfarnesane	1.17E+02	1.39E+02	1.01E+02	<350	6.93E+02	<350	2.33E+04	1.16E+05	1.36E+04	2.27E+04	0.257	<75	1.31E+02	1.10E+03
farnesane	2.97E+02	3.01E+02	2.30E+02	1.69E+03	5.11E+02	4.84E+02	1.32E+04	<6000	<8000	<15000	<0.02	4.79E+02	1.61E+02	8.05E+01
tetradecane	3.61E+03	3.49E+03	3.14E+03	1.39E+04	1.80E+04	1.44E+04	2.70E+05	1.73E+05	2.38E+05	4.75E+05	0.327	2.88E+03	3.49E+03	2.58E+03
pentadecane	2.12E+03	1.95E+03	1.84E+03	5.15E+03	7.85E+03	4.81E+03	1.93E+05	1.21E+05	1.19E+05	3.34E+05	0.219	2.54E+03	2.68E+03	2.60E+03
hexadecane	3.72E+03	3.84E+03	3.48E+03	1.13E+04	1.35E+04	1.25E+04	3.04E+05	2.09E+05	2.28E+05	5.58E+05	0.352	3.49E+03	3.59E+03	3.40E+03
norpristane	4.06E+02	3.79E+02	3.88E+02	2.45E+03	2.30E+03	4.19E+03	4.26E+04	3.23E+04	3.76E+04	8.17E+04	0.042	4.34E+02	1.54E+02	3.59E+02
heptadecane	3.38E+03	3.66E+03	3.32E+03	7.85E+03	1.01E+04	7.52E+03	2.72E+05	1.97E+05	1.83E+05	5.87E+05	0.364	2.97E+03	1.95E+03	2.16E+04
octadecane	2.07E+03	2.16E+03	2.16E+03	4.66E+03	5.33E+03	3.61E+03	9.43E+04	5.11E+04	5.04E+04	1.29E+05	0.075	3.13E+03	2.54E+03	1.54E+03
nonadecane	2.07E+03	2.20E+03	1.97E+03	2.58E+03	2.99E+03	2.65E+03	8.22E+04	5.52E+04	5.52E+04	1.95E+05	0.123	2.61E+03	2.83E+03	2.56E+03
tritriacontane	1.59E+04	1.62E+04	1.81E+04	2.27E+04	2.13E+04	2.27E+04	5.88E+04	4.52E+04	5.36E+04	1.15E+05	0.062	2.06E+04	1.80E+04	1.78E+04
tetratriacontane	6.01E+03	6.55E+03	6.09E+03	4.45E+03	4.56E+03	5.55E+03	7.30E+04	<6000	3.04E+04	8.12E+05	0.391	6.66E+03	6.28E+03	5.86E+03
pentatriacontane	3.58E+03	5.15E+03	6.01E+03	3.83E+03	3.10E+03	3.90E+03	2.64E+04	2.11E+04	2.64E+04	4.99E+04	0.042	5.18E+03	5.09E+03	4.90E+03
hexatriacontane	3.57E+03	4.00E+03	2.67E+03	2.24E+03	2.99E+03	3.77E+03	4.87E+04	1.58E+04	4.32E+04	1.09E+05	0.094	3.93E+03	1.91E+03	3.87E+03
heptatriacontane	2.43E+03	3.43E+03	2.79E+03	2.06E+03	1.86E+03	2.65E+03	2.33E+04	1.29E+04	<8000	3.48E+04	0.027	3.17E+03	2.77E+03	2.47E+03
octatriacontane	1.61E+03	1.98E+03	1.95E+03	1.90E+03	1.64E+03	3.13E+03	2.74E+04	1.12E+04	1.84E+04	4.24E+04	0.047	2.14E+03	1.40E+03	2.04E+03
nonatriacontane	1.23E+03	1.77E+03	1.74E+03	1.07E+03	8.39E+02	1.68E+03	1.01E+04	8.80E+03	1.28E+04	3.33E+04	0.022	1.39E+03	7.92E+02	1.49E+03

11 cont	Additional PAH (In chromatographic elution order)														
	2-methylnaphthalene	8.67E+02	8.27E+02	7.97E+02	1.72E+03	1.75E+03	1.58E+03	5.88E+04	4.23E+04	4.40E+04	1.03E+05	0.072	8.75E+02	8.46E+02	1.01E+03
	1-methylnaphthalene	6.17E+02	5.41E+02	5.46E+02	9.51E+02	1.02E+03	8.39E+02	3.14E+04	2.41E+04	2.40E+04	6.51E+04	0.041	1.51E+03	1.38E+03	2.01E+03
	Biphenyl	2.42E+02	2.24E+02	2.08E+02	4.60E+02	5.47E+02	4.52E+02	1.42E+04	7.04E+03	1.12E+04	1.97E+04	<0.02	1.90E+02	1.84E+02	2.12E+02
	1+2ethylnaphthalene	2.97E+02	2.70E+02	2.66E+02	4.60E+02	6.57E+02	4.19E+02	1.52E+04	1.17E+04	1.28E+04	2.72E+04	<0.02	2.97E+02	2.46E+02	3.66E+02
	2,6+2,7-dimethylnaphthalene	3.83E+02	3.94E+02	4.09E+02	3.68E+02	5.11E+02	3.55E+02	1.52E+04	<6000	8.81E+03	<15000	<0.02	4.49E+02	4.61E+02	4.61E+02
	1,3+1,6+1,7dimethylnaphth	1.02E+03	1.02E+03	9.76E+02	7.36E+02	7.30E+02	6.45E+02	2.23E+04	1.82E+04	1.60E+04	4.08E+04	0.028	1.44E+03	1.51E+03	1.49E+03
	1,4+1,5+2,3-dimethylnaphth	5.86E+02	5.18E+02	4.95E+02	<350	4.74E+02	<350	1.01E+04	9.98E+03	8.81E+03	1.66E+04	<0.02	3.65E+02	3.15E+02	4.17E+02
	1,2-dimethylnaphthalene	3.83E+02	2.94E+02	3.59E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	4.64E+02	3.61E+02	5.49E+02
	2-Methylbiphenyl	1.56E+02	1.24E+02	1.44E+02	<350	5.11E+02	4.19E+02	<10000	6.46E+03	<8000	<15000	<0.02	2.66E+02	1.92E+02	1.83E+02
	3-Methylbiphenyl	2.03E+02	2.78E+02	2.08E+02	6.44E+02	5.84E+02	<350	1.32E+04	6.46E+03	1.04E+04	2.12E+04	<0.02	2.74E+02	3.31E+02	3.00E+02
	4-Methylbiphenyl	3.20E+02	3.09E+02	2.87E+02	1.04E+03	1.28E+03	1.03E+03	<10000	<6000	<8000	<15000	<0.02	3.96E+02	3.46E+02	1.54E+02
	Dibenzofuran	4.77E+02	4.71E+02	4.67E+02	4.91E+02	5.47E+02	5.16E+02	1.42E+04	8.80E+03	1.04E+04	2.27E+04	<0.02	3.42E+02	3.23E+02	3.15E+02
	Bibenzyl	1.41E+02	1.55E+02	1.87E+02	1.04E+03	1.64E+03	1.42E+03	1.01E+05	5.40E+04	4.48E+04	7.26E+04	0.088	1.52E+02	2.92E+02	2.64E+02
	A-trimethylnaphthalene	2.27E+02	2.32E+02	2.23E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.67E+02	1.92E+02	2.71E+02
	1-ethyl-2-methylnaphth	1.02E+02	8.50E+01	1.08E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.67E+02	1.46E+02	1.61E+02
	B-trimethylnaphthalene	2.11E+02	2.24E+02	2.08E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.90E+02	1.92E+02	1.68E+02
	C-trimethylnaphthalene	2.42E+02	2.32E+02	2.58E+02	<350	6.57E+02	<350	<10000	<6000	<8000	<15000	<0.02	2.36E+02	2.23E+02	2.20E+02
	2-ethyl-1-methylnaphth	1.17E+02	9.27E+01	1.08E+02	<350	6.20E+02	<350	<10000	<6000	<8000	<15000	<0.02	2.97E+02	3.15E+02	1.32E+02
	E-trimethylnaphthalene	2.58E+02	2.24E+02	2.44E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.89E+02	2.46E+02	3.00E+02
	F-trimethylnaphthalene	1.64E+02	1.39E+02	1.72E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.66E+02	5.38E+02	3.00E+02
	2,3,5+I-trimethylnaphthalene	2.50E+02	2.32E+02	2.23E+02	<350	<350	6.77E+02	<10000	<6000	<8000	<15000	<0.02	1.98E+02	2.84E+02	2.49E+02
	2,4,5-trimethylnaphthalene	9.38E+01	1.31E+02	2.44E+02	<350	<350	4.84E+02	<10000	7.63E+03	<8000	<15000	<0.02	2.82E+02	2.15E+02	4.98E+02
	J-trimethylnaphthalene	9.38E+01	9.27E+01	8.61E+01	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	<80	<80	<80
	1,4,5-trimethylnaphthalene	<80	<80	1.15E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	<80	<80	<80
	Acenaphthylene	3.44E+02	3.63E+02	3.66E+02	<350	4.01E+02	<350	<10000	8.22E+03	<8000	<15000	<0.02	2.97E+02	3.61E+02	3.44E+02
	Acenaphthene	1.56E+02	1.78E+02	1.51E+02	<350	4.01E+02	<350	<10000	<6000	<8000	<15000	<0.02	2.66E+02	2.08E+02	1.46E+02
	dibenzothiophene	6.95E+02	7.03E+02	7.75E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	5.02E+02	6.23E+02	6.08E+02
	A-methylfluorene	<80	3.09E+02	1.22E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.22E+02	1.38E+02	1.17E+02
	1-methylfluorene	1.17E+02	1.16E+02	1.15E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.22E+02	1.31E+02	1.24E+02
	B-methylfluorene	<80	<80	1.08E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	<80	<80	<80
	Xanthone	1.41E+02	1.24E+02	1.22E+02	<350	6.20E+02	<350	1.01E+04	<6000	<8000	<15000	<0.02	1.75E+02	1.54E+02	1.61E+02
	2-methlyanthracene	2.27E+02	1.85E+02	2.66E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.21E+02	2.31E+02	1.68E+02
	4,5-dimethylphenanthrene	3.67E+02	3.63E+02	4.02E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.89E+02	3.15E+02	2.86E+02
	Anthrone	2.50E+02	2.32E+02	3.59E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	<80	1.23E+02	8.05E+01
	3,6-dimethylphenanthrene	1.72E+02	1.70E+02	2.15E+02	<350	<350	3.55E+02	1.12E+04	<6000	<8000	<15000	0.026	1.83E+02	1.61E+02	1.46E+02
	A-dimethylphenanthrene	3.59E+02	3.48E+02	3.88E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	3.50E+02	3.00E+02	3.73E+02
	B-dimethylphenanthrene	2.34E+02	2.24E+02	2.37E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.45E+02	1.54E+02	1.46E+02
	C-dimethylphenanthrene	5.47E+02	5.72E+02	6.10E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	5.48E+02	5.84E+02	5.42E+02
	D-dimethylphenanthrene	2.50E+02	2.70E+02	2.66E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.82E+02	3.23E+02	2.71E+02
	1,7-dimethylphenanthrene	3.91E+02	3.94E+02	2.08E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	4.79E+02	2.61E+02	4.25E+02
	E-dimethylphenanthrene	2.66E+02	2.70E+02	3.09E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.14E+02	2.69E+02	2.05E+02
	9-methylanthracene	1.25E+02	<80	<80	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.13E+02	2.31E+02	1.90E+02

11 cont	9-Anthraaldehyde	2.27E+02	1.39E+02	1.08E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.07E+02	2.31E+02	<80	
	Benzonephthothiophene	2.23E+03	2.27E+03	2.31E+03	3.99E+02	4.38E+02	4.19E+02	1.12E+04	6.46E+03	<8000	<15000	<0.02	1.45E+03	1.38E+03		1.43E+03
	1+3-methylfluoranthene	6.56E+02	2.16E+02	1.44E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	3.73E+02	4.92E+02		1.83E+02
	1-MeFl+C-MeFl/Py	2.66E+02	2.16E+02	2.15E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	4.57E+02	4.15E+02		2.86E+02
	B-MePy/MeFl	6.56E+02	2.16E+02	1.44E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	3.12E+02	4.92E+02		6.66E+02
	C-MePy/MeFl	1.80E+02	2.94E+02	3.23E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	2.66E+02	2.54E+02		3.15E+02
	D-MePy/MeFl	7.58E+02	6.80E+02	8.11E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	5.33E+02	4.69E+02		5.64E+02
	4-methylpyrene	5.55E+02	5.95E+02	5.96E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	5.18E+02	3.61E+02		4.54E+02
	1-methylpyrene	3.44E+02	3.32E+02	3.73E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	3.50E+02	3.46E+02		2.49E+02
	Benzo(c)phenanthrene	3.36E+02	3.40E+02	3.23E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.14E+02	2.08E+02		2.05E+02
	7-methylbenz(a)anthrecene	<80	<80	<80	<350	<350	<350	1.12E+04	7.04E+03	<8000	<15000	<0.02	<80	<80	<80	
	3-methylchrysene	2.73E+02	1.24E+02	2.37E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.29E+02	2.23E+02		1.83E+02
	5+6-methylchrysene	<80	<80	<80	<350	<350	<350	1.93E+04	1.29E+04	8.81E+03	<15000	<0.02	<80	<80	<80	
	Benzo(b+j+k)fluoranthene	1.81E+04	1.85E+04	1.85E+04	2.21E+03	2.23E+03	2.03E+03	6.39E+04	4.52E+04	3.76E+04	4.54E+04	0.072	9.48E+03	1.09E+04		1.08E+04
	Benzo(e)fluoranthene	1.72E+02	1.70E+02	2.01E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	1.52E+02	1.08E+02		1.68E+02
	7-methylbenzo(e)pyrene	1.56E+02	1.39E+02	2.51E+02	<350	<350	<350	1.83E+04	1.17E+04	1.04E+04	1.97E+04	0.034	<80	<80	<80	
	Dibenzo(e,j)anthracene	2.97E+02	3.25E+02	2.80E+02	<350	<350	<350	<10000	<6000	<8000	<15000	<0.02	5.78E+02	4.61E+02		2.27E+02
	Dibenzo(eh+ac)enthracene	1.30E+03	7.19E+02	1.21E+03	5.83E+02	6.93E+02	5.48E+02	3.25E+04	2.35E+04	1.84E+04	2.27E+04	0.03	7.76E+02	9.76E+02		4.39E+02
	Picene	9.84E+02	7.19E+02	1.11E+03	4.60E+02	4.74E+02	<350	<10000	1.23E+04	1.20E+04	1.66E+04	<0.02	3.73E+02	5.00E+02		3.73E+02
	Anthanthrene	<80	<80	<80	4.29E+02	<350	3.87E+02	1.42E+04	8.80E+03	8.81E+03	<15000	<0.02	8.37E+01	<80	<80	
	Dibenzo(b,k)fluorenthene	2.83E+03	3.52E+03	2.15E+03	1.17E+03	1.93E+03	1.19E+03	3.04E+04	1.82E+04	8.01E+03	1.82E+04	<0.02	2.75E+03	7.15E+02		2.03E+03
	Dibenzo(e,h)pyrene	1.02E+02	2.86E+02	<80	3.07E+02	6.57E+02	5.16E+02	1.12E+04	<6000	<8000	<15000	<0.02	<80	<80	<80	
	Additionel acids, phenols, and sterols (in chrometographic elution order)															
	Sterols, phenols, acids, and sugars are analyzed as TMS derivatives in one GC-ITD method. Derivatization is done with a mixture of BSTFA + 1% TMCS and pyridine (3:1), acetonitrile. Calibration solutions were freshly derivatized on same analytical day with analytes.															
	heptanoic acid	1.21E+04	1.11E+04	1.16E+04	2.78E+04	1.45E+04	2.20E+04	4.31E+05	2.27E+05	2.85E+05	7.29E+05	0.771	1.88E+04	1.74E+04		1.70E+04
	benzoic acid	2.18E+04	2.27E+04	2.03E+04	5.07E+04	9.45E+04	9.46E+04	3.04E+06	1.90E+06	2.31E+06	4.47E+06	4.088	1.67E+04	1.48E+04		1.00E+04
	octenoic acid	2.63E+04	2.54E+04	2.57E+04	6.23E+04	3.23E+04	4.92E+04	1.38E+06	5.67E+05	7.06E+05	2.04E+06	1.812	3.27E+04	3.14E+04		3.18E+04
	phenylacetic acid	2.34E+02	3.09E+02	2.08E+02	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	3.81E+02	4.30E+02		4.39E+02
	meleic acid	4.98E+03	5.49E+03	5.03E+03	6.67E+04	5.89E+04	5.04E+04	8.41E+06	3.34E+06	4.26E+06	1.08E+07	5.894*	3.30E+04	4.23E+04		4.64E+04
	succinic acid	4.01E+04	3.76E+04	3.87E+04	6.17E+04	6.44E+04	5.94E+04	6.21E+06	2.06E+06	2.15E+06	1.16E+07	13.598*	1.55E+05	1.24E+05		1.17E+05
	me-succinic acid	9.01E+03	8.77E+03	8.97E+03	1.20E+04	1.28E+04	8.55E+03	1.38E+06	3.52E+05	3.66E+05	1.59E+06	1.175*	3.36E+04	2.54E+04		2.42E+04
	o-toluic	3.20E+02	4.17E+02	3.37E+02	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	5.02E+02	5.61E+02		6.00E+02
	m-toluic	1.13E+03	1.14E+03	1.06E+03	8.28E+02	<730	8.06E+02	2.43E+04	1.29E+04	1.92E+04	4.54E+04	<0.04	1.92E+03	1.94E+03		1.90E+03
	nonenoic acid	4.61E+04	4.02E+04	4.33E+04	1.27E+05	7.77E+04	8.51E+04	3.94E+06	1.58E+06	1.97E+06	5.70E+06	5.234	3.18E+04	3.36E+04		3.31E+04
	p-toluic	8.28E+02	8.35E+02	8.26E+02	8.59E+02	1.13E+03	7.42E+02	2.74E+04	1.35E+04	<16000	3.93E+04	<0.04	1.67E+03	1.54E+03		1.55E+03
	2,6-dimethylbenzoic acid	<150	<150	<150	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	<150	<150	<150	
	giuteric acid	1.34E+04	1.46E+04	1.48E+04	2.79E+04	2.59E+04	2.20E+04	1.50E+06	7.39E+05	6.00E+05	2.71E+06	2.75*	4.04E+04	4.32E+04		3.88E+04
	2-methylgluteric	3.44E+03	3.49E+03	4.12E+03	2.09E+03	<730	9.68E+02	2.60E+05	1.96E+05	<16000	3.27E+05	1.02*	9.39E+03	1.02E+04		9.49E+03
	2,5-dimethylbenzoic acid	2.66E+02	4.02E+02	3.09E+02	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	4.11E+02	4.30E+02		4.76E+02
	3-methylgluteric acid	3.14E+03	3.78E+03	3.55E+03	3.65E+03	<730	1.39E+03	5.60E+05	<11000	<16000	<30000	<0.04	8.08E+03	9.41E+03		9.09E+03
	2,4-dimethylbenzoic acid	7.19E+02	8.11E+02	7.75E+02	1.26E+03	2.19E+03	1.45E+03	7.40E+04	3.29E+04	4.40E+04	1.16E+05	0.063	9.82E+02	9.38E+02		9.74E+02
	2,3- end 3,5-dimethylbenzoic acid	3.28E+02	4.56E+02	4.59E+02	6.44E+02	<730	<650	3.14E+04	<11000	1.76E+04	3.78E+04	<0.04	5.78E+02	5.00E+02		5.49E+02
	decanoic acid	3.15E+03	2.40E+03	2.97E+03	5.74E+03	6.09E+03	4.90E+03	1.48E+05	7.92E+04	1.02E+05	2.42E+05	0.128	3.01E+03	4.71E+03		3.28E+03
	4-allyl-guaiacol (eugenol)	<150	<150	<150	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	<150	<150		2.93E+02
	4-methyl-syringol	<150	<150	<150	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	<150	<150	<150	
	3,4-dimethylbenzoic acid	6.33E+02	9.58E+02	8.69E+02	1.72E+03	2.08E+03	1.00E+03	<20000	<11000	<16000	<30000	<0.04	1.10E+03	1.18E+03		1.22E+03
	hexanedioic (edipic) acid	7.63E+03	6.28E+03	6.63E+03	1.48E+04	2.32E+04	1.25E+04	1.86E+06	7.95E+05	5.75E+05	2.97E+06	10.696*	1.66E+04	1.45E+04		1.72E+04
	cis-pinonic acid	2.03E+02	4.17E+02	1.72E+02	9.20E+02	<730	7.10E+02	2.74E+04	1.58E+04	2.00E+04	5.45E+04	<0.04	<150	5.76E+02		8.64E+02
	salcylic acid	1.36E+03	2.83E+03	2.79E+03	1.84E+03	1.79E+03	1.58E+03	2.94E+04	2.17E+04	2.32E+04	4.54E+04	<0.04	1.47E+03	3.87E+03		3.37E+03
	3-methyladipic acid	1.31E+03	1.31E+03	1.89E+03	<600	<730	<650	<20000	4.64E+04	<16000	1.60E+05	0.782*	2.64E+03	3.19E+03		4.08E+03
	4-formyl-guelacol (venillin)	1.50E+03	1.60E+03	1.92E+03	4.94E+03	5.15E+03	4.39E+03	1.08E+05	5.63E+04	7.53E+04	1.42E+05	0.074	1.29E+03	1.26E+03		1.24E+03

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	undecanoic acid	2.55E+03	2.20E+03	2.50E+03	4.29E+03	4.16E+03	3.90E+03	1.03E+05	5.46E+04	7.13E+04	1.48E+05	0.092	3.36E+03	4.54E+03		3.95E+03
	heptanedioic (pimelic) acid	3.80E+03	4.59E+03	3.89E+03	1.04E+04	8.14E+03	8.45E+03	5.03E+05	<11000	2.33E+05	1.01E+06	4.009*	1.85E+04	1.48E+04		1.98E+04
	2,3-dimethoxybenzoic acid	1.31E+04	4.26E+03	3.35E+03	<600	<730	<650	<20000	<11000	<16000	6.96E+04	<0.04	4.16E+03	6.68E+03		5.18E+03
	acetovanillone	2.50E+02	8.96E+02	5.24E+02	9.51E+02	<730	<650	<20000	<11000	<16000	<30000	<0.04	5.40E+02	<150		1.22E+03
	2,6-dimethoxybenzoic acid	<150	<150	1.65E+02	<600	<730	<650	2.13E+04	<11000	<16000	8.17E+04	<0.04	<150	1.07E+03	<150	
	dodecanoic (lauric) acid	1.53E+04	1.26E+04	1.54E+04	2.12E+04	5.64E+04	1.70E+04	6.55E+05	2.46E+05	2.79E+05	8.35E+05	0.496	1.03E+04	2.42E+04		1.16E+04
	2,5-dimethoxybenzoic acid	<150	3.40E+02	<150	<600	<730	<650	<20000	<11000	<16000	4.84E+04	<0.04	<150	<150	<150	
	phthalic acid	2.03E+02	3.86E+03	1.29E+04	1.82E+04	1.56E+04	1.18E+04	5.75E+05	3.47E+05	3.39E+05	8.37E+05	2.252*	1.39E+05	7.47E+04		5.33E+04
	suberic acid	<150	<150	3.28E+04	<600	<730	4.58E+03	9.23E+04	<11000	8.73E+04	4.08E+05	1.988*	3.83E+04	1.39E+04		2.21E+04
	3,5-dimethoxybenzoic acid	<150	1.01E+03	9.98E+02	<600	<730	1.84E+03	<20000	<11000	1.84E+04	4.99E+04	<0.04	<150	<150	<150	
	syringaldehyde	9.62E+03	3.66E+03	2.46E+03	5.98E+03	5.33E+03	5.94E+03	<20000	<11000	<16000	3.63E+04	<0.04	1.75E+03	2.38E+03		2.45E+03
	3,4-dimethoxybenzoic acid	5.13E+03	2.94E+03	1.73E+03	1.50E+03	<730	1.58E+03	<20000	<11000	<16000	6.66E+04	<0.04	2.05E+03	2.86E+03		3.68E+03
	2,4-dimethoxybenzoic acid	<150	<150	<150	<800	<730	<650	<20000	<11000	<16000	6.96E+04	<0.04	5.94E+02	<150		9.52E+02
	tridecanoic acid	2.41E+03	2.13E+03	2.35E+03	3.25E+03	3.72E+03	3.06E+03	7.00E+04	3.81E+04	4.72E+04	9.98E+04	0.062	3.76E+03	3.62E+03		3.82E+03
	isophthalic acid	1.45E+04	3.40E+03	7.40E+03	3.37E+03	1.58E+04	4.61E+03	2.21E+05	9.04E+04	1.36E+05	4.19E+05	1.448*	1.69E+04	1.43E+04		9.08E+03
	vanlilic acid	2.94E+04	1.43E+04	8.61E+03	1.82E+04	2.50E+04	2.41E+04	8.22E+04	4.81E+04	8.89E+04	1.54E+05	0.139	1.57E+04	2.19E+04		2.63E+04
	homovanlilic acid	6.17E+03	8.71E+03	1.24E+04	1.76E+04	5.22E+04	6.62E+04	1.66E+06	3.12E+05	2.55E+05	8.96E+05	1.988	3.98E+03	2.58E+03		3.77E+03
	azelaic acid	2.16E+05	5.60E+04	1.52E+05	3.31E+04	4.23E+04	3.10E+04	6.71E+05	4.74E+05	7.02E+05	3.11E+06	2.646*	2.68E+05	1.75E+05		1.34E+05
	myristoleic acid	<150	<150	<150	<800	<730	<650	<20000	<11000	<16000	<30000	<0.04	<150	<150	<150	
	myristic acid	2.78E+04	2.57E+04	2.45E+04	2.84E+04	3.77E+04	3.09E+04	7.23E+05	3.94E+05	4.79E+05	1.05E+06	0.654	3.83E+04	3.95E+04		3.65E+04
	sebacic acid	2.38E+04	7.79E+03	2.00E+04	6.07E+03	6.50E+03	6.23E+03	1.30E+05	6.16E+04	9.05E+04	3.69E+05	0.521	3.52E+04	2.01E+04		1.66E+04
	syringic acid	4.68E+03	3.15E+03	1.63E+03	1.10E+03	2.23E+03	2.03E+03	<20000	<11000	<16000	<30000	<0.04	2.25E+03	1.32E+03		2.58E+03
	pentadecanoic acid	7.27E+03	8.15E+03	7.09E+03	1.10E+04	1.12E+04	1.00E+04	1.33E+05	8.33E+04	1.17E+05	2.28E+05	0.138	1.71E+04	1.45E+04		1.45E+04
	undecanedioic acid	3.67E+03	3.72E+03	5.28E+03	2.58E+03	4.93E+03	3.29E+03	6.44E+05	3.70E+04	5.60E+04	1.69E+05	1.21*	8.08E+03	2.41E+04		7.96E+03
	palmitoleic acid	2.18E+03	3.15E+03	2.48E+03	1.44E+03	2.70E+03	2.26E+03	2.64E+04	1.70E+04	<16000	5.60E+04	0.015	1.60E+03	2.05E+03		1.78E+03
	isostearic acid	<150	<150	<150	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	<150	1.84E+02	<150	
	dodecanedioic acid	7.11E+02	6.80E+02	7.61E+02	6.75E+02	1.28E+03	9.03E+02	1.80E+05	1.29E+04	1.60E+04	5.75E+04	0.52	1.42E+03	2.18E+03		1.26E+03
	heptadecanoic acid	1.27E+04	1.56E+04	1.49E+04	1.01E+04	1.08E+04	1.15E+04	1.41E+05	1.16E+05	1.51E+05	2.89E+05	0.15	3.11E+04	2.15E+04		2.77E+04
	oleic acid	6.99E+04	4.95E+04	4.91E+04	2.19E+04	4.66E+04	6.01E+04	<20000	7.45E+04	2.75E+05	<30000	0.112	9.71E+04	7.59E+04		6.73E+04
	elaidic acid	5.19E+03	5.05E+03	4.90E+03	3.56E+03	6.93E+03	6.52E+03	8.92E+04	6.51E+04	1.18E+05	1.53E+05	0.104	9.80E+03	8.34E+03		8.98E+03
	stearic acid	2.94E+05	2.25E+05	2.76E+05	7.19E+04	1.55E+05	2.01E+05	3.19E+06	2.41E+06	3.01E+06	6.67E+06	3.985	3.22E+05	4.86E+05		3.05E+05
	8,15-pimaradien-18-oic acid	5.16E+02	3.71E+02	2.66E+02	8.90E+02	<730	1.45E+03	2.33E+04	1.29E+04	<16000	3.93E+04	<0.04	5.78E+02	9.15E+02	<150	
	nonadecanoic acid	7.76E+03	6.88E+03	7.47E+03	7.33E+03	6.93E+03	7.10E+03	3.14E+04	3.11E+04	4.00E+04	6.20E+04	<0.04	1.47E+04	1.72E+04		1.50E+04
	sandaracopimaric	<150	<150	<150	1.99E+03	3.07E+03	2.32E+03	<20000	<11000	<16000	<30000	<0.04	<150	<150	<150	
	paulustric acid	<150	<150	2.76E+03	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	<150	<150		4.41E+03
	dihydroisopimaric acid	<150	<150	<150	<600	<730	<850	<20000	<11000	<16000	<30000	<0.04	<150	2.69E+02	<150	
	8-abietic acid	2.42E+02	<150	<150	<600	<730	<650	<20000	<11000	<16000	<30000	<0.04	2.51E+02	<150	<150	
	dehydroabietic acid	1.96E+04	1.67E+04	1.87E+04	5.77E+03	4.42E+03	5.45E+03	6.90E+04	3.99E+04	5.28E+04	1.18E+05	<0.04	1.56E+04	1.80E+04		1.45E+04
	eicosanoic acid	1.25E+04	1.16E+04	1.28E+04	2.71E+04	2.57E+04	2.67E+04	1.26E+05	6.92E+04	9.61E+04	1.59E+05	<0.04	2.18E+04	1.68E+04		2.14E+04
	abietic acid	<150	<150	<150	<600	<730	5.16E+02	<20000	<11000	<16000	<30000	<0.04	<150	<150	<150	
	heneicosanoic acid	1.40E+04	1.32E+04	1.52E+04	2.44E+04	2.16E+04	2.32E+04	4.06E+04	3.93E+04	7.29E+04	1.06E+05	<0.04	3.09E+04	1.83E+04		3.23E+04
	7-oxodehydroabietic acid	7.35E+04	5.58E+04	7.19E+04	1.99E+04	2.23E+04	3.25E+04	6.31E+05	1.67E+05	1.86E+05	3.80E+05	0.143	1.58E+05	<150		1.63E+05
	docosanoic acid	8.86E+04	7.55E+04	8.97E+04	2.10E+05	1.88E+05	2.36E+05	<20000	2.71E+05	<16000	5.96E+05	0.114	1.36E+05	9.02E+04		1.40E+05
	tricosanoic acid	2.86E+04	2.36E+04	2.72E+04	5.87E+04	4.94E+04	5.55E+04	6.80E+04	7.34E+04	1.48E+05	1.62E+05	<0.04	5.06E+04	2.21E+04		5.50E+04
	tetracosanoic acid	2.15E+05	1.96E+05	2.06E+05	4.88E+05	4.01E+05	4.45E+05	3.58E+05	5.23E+05	7.93E+05	1.06E+06	0.135	3.07E+05	1.19E+05		4.23E+05
	b-sitosterol	3.89E+04	3.11E+04	2.18E+04	1.32E+05	3.69E+04	7.42E+04	2.53E+05	2.01E+05	1.41E+05	7.84E+05	0.488	1.50E+04	<150		1.85E+04
	*cmpds with poor internal std abundance															

Appendix C

Laboratory Methods Used

Lab #	g extracted SRM 168	g extracted Balt-2 PM	µg extracted RM 8785	g extracted SRM 1649a	Extraction Method	Extraction Solvent	Extraction Time	Extraction other
1a	0.06	0.03	638 - 2282	0.06	PFE	dichloromethane	3 cycles at 5 min each	100 °C; 2000 psi; 3 cylces of 5 min static; flush 90%; purge 180 sec
1b	0.018	0.027	608-1396		PFE	dichloromethane	three cycles at 2000 psi and 100 C	solid phase: hydromatrix
1c					PFE	dichloromethane	3 cycles at 5 min cach	100 °C; 2000 psi; 3 cycles of 5 min static;
2	0.07	0.07	646-2284	0.07	sonication	20 mL dichloromethane:methanol (9:1)	20 min	
3a			663-2001	0.01	PFE	dichloromethanc	60 min	100 °C
3b			626-1417	0.02	sonication	2 x 5 ml cyclohexane/CH2Cl2 (4:1)	2 x 45 min	
4			673-2007	0.5	PFE	acetone:dichloromethane (1:4)	Heat = 5 s ; Static = 5 s ; Purge = 300 s	T = 100 °C; P = 1500 psi; flush= 60%; 4 cycles
5	0.1	0.1		0.1	PFE	dichloromethane:ethyl acetate (3:1)		40 °C, 1500 psi, static 5 min, flush 60%, cycle 2, purge 60 sec
6	0.3	0.09		0.3	sonication	dichloromethane	1.5 h	
7	0.1	0.03	659-1673	0.1	microwave assisted cxtraction	acetone:hexane (1:1)	10 min	
8	0.1	0.02	490-1064	0.01	Soxhlet	toluene	24 h	
9	0.05	0.03	696-1682	0.05	PFE	toluene	Heating time 7 min, static extraction 5 min, three cycles	100°C, 1500 psi, 3 cycles
10	0.03	0.03	509-1482	0.03	PFE (2 times)	dichloromethane	5-min heat up and 5-min static; Nitrogen purge for 180 seconds	Cell pressure @ temperature: 2000 psi @ 100°C; Nitrogen purge at 100 psi for 240 sec
11	0.13	0.03	661-1704	0.13	PFE	dichloromethane then acetone	20 min per solvent	80 °C with 1500 psi
12	0.007	0.007	314-1288	0.007	Sonication	30 ml hexane (2x), 20 ml benzene/IPA (3x)		
14	0.006	0.006	577-1385	0.006	Sonication	dichloromethane:acetonitrile (2:1)	24 min	

Lab #	Sample extract cleanup method	Method of quantitation
1a	conc with solvent change to hexanc for dichloromethane extracts; aminopropyl solid phase extraction (SPE) column; condition and clutc with 40 mL of 20 % dichloromethane in hexane; to isolate nitroPAHs - semiprcparative amino/cyano HPLC fractionation	IS
1b	2 % methylene chloride in hcxanc with silica plus sep-pak cartridges (15 mL mobile phase)	IS
1c	aminopropyl solid phase extraction (SPE) column; condition and elute with 15 mL of 10 % dichloromethane in hexane	IS
2	Fluorisil SPE cleanup; silicagcl 6 g column; filter 0.45 µm prior to analysis	ES
3a	solvent is cxhanged to acetonitrile and thc final extract is filtered through Gclman GHP Bulk Acrodisk Syringe Filter 0.45 µm	ES
3b	Thc cxtracts wcre centrifugcd and evaporated (TurboVap 37 C) under nitrogen to final volume in cyclohexane. The final volume was 1 ml (SRM 1649a), 300 µl (filter 1 and blank filter) or 150 µl (filters 2, 3 and 4).	IS
4	Neutral alumina column with isooctane/dichlomethane mixture (21 ml, 1:2).	IS
5	Silica gel chromatography; fraction 1-n-alkanes, 25mL of hexane; fraction 3- ketones and quinones: 25mL of hexanc to ethyl acetate, 5:1, v/v; fraction 4- acids +sugar, 30mL of ethyl acetate to mthanol, 3:1, v/v	IS and ES
6	SPE cartridges of two types were used: Cyanopropyl and silica (Alltech, 500 mg/4 mL). Cyanopropyl cartridge was preconditioned using 4 mL of hexane. Samples were eluted with hexane 1.5 mL (fraction 1) followed of hexane:dichloromethane mixture 1:1, 1.5 mL (fraction 2). The extract of fraction 1 was refractioned into silica cartridge preconditioned with hexane 4 mL using hexane 1.5 mL (fraction 1a) followed by dichlromethane 1.5 mL (fraction 1b).	IS
7	split: PAH silica column; nPAH: liq/liq DMSO then HPLC	IS
8	DMF/water (9:1) / cyclohexane; HPLC fractionation: NUCLEOSIL 50 5µm L: 250 mm ID: 8 mm - hexane/dichloromethane	IS
9	evaporation using DMF as keeper, dissolution in acetonitrile for HPLC-analysis; injection of an amount of toluene extract for GC/MS-analysis	ES
10	Dichloromethane extracts were subjected to solvent exchange to hexane prior to chromatographic separation. The chromatographic separations were performed on a 5% (w/w) water deactivated silica column. The n-paraffins/biomarkers fraction was obtained by eluting 15 mL hexane.	IS
11	NA	IS
12	filtration	IS
14	filtering . 0.45 µm filters	ES

Lab #	Instrument	**PAHs** Phase	Calibration Curve Dimensions	# points	range
1a	GC/EI-MS	DB-17MS	30m x 0.25 mm, 0.25µm film	5	100 - 10000 ng/g
1b	GC/MS	DB-17 MS	60m x 0.25 mm, 0.25µm film	6	0.5 - 110 ng extracted
1c	GC/MS	DB-17	60m x 0.25 mm, 0.25µm film	5	0.04 - 4 ug/mL
2	HPLC FLD	PAH C18	0.25m x 4.6 mm, 5µm film	9	1- 1000 ng/mL
3a	HPLC FLD	ChromSpher PAH	0.01m x 3 mm, 3µm film	6	1:500 - 1:80 dilutions
3b	GC/MS	DB-17MS	30m x 0.25 mm, 0.25µm film	6	1 - 200 pg/µL
4	GC/EI-MS	HP-5MS	30m x 0.25 mm, 0.25µm film	3	0.5 - 15 ng/µL
6	GC/MS	5% phenyl	29m x 0.25 mm, 0.25µm film	7	0.06 - 10.727 µg/mL
7	GC/MS	DB-XLB	30m x 0.25 mm, 0.25µm film	7	0.01 - 25 ng/µL
8	GC/EI-MS	1)CPSil5MS 2)DB17MS	0m x 0.25 mm, 0.25µm film (1) or 0.15 µm film (2	9	0.03 - 10 ng injected
9	HPLC-FD / GC-TOF-MS	RP-18, 5 µm / Thermo TR-5MS	0.25m x 3 mm / 15m x 0.25 mm, 0.25µm film	6	2 - 1000 pg/µL
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	6	0.1-10 ng/µL
12	GC/MS	HP-5MS	60m x 0.25 mm, 0.25µm film	5	0.5-5 ng/µL
14	HPLC FLD	LC-18	0.15m x 4.6 mm, 5µm film	5	10-500ppb

Lab #	Instrument	**Nitro-PAHs** Phase	Calibration Curve Dimensions	# points	range
1a	GC/NCI-MS	DB-17 MS	30m x 0.25 mm, 0.25µm film	5	10 - 500 ng/g
4	GC/NCI-MS	DB-17 MS	30m x 0.25 mm, 0.25µm film	3	0.5 - 3 ng/µL
7	HRGC/HRMS	DB-5	60m x 0.25 mm, 0.25µm film	4	0.7 - 11 ng/µL

Lab #	Instrument	**PAH-quinone** Phase	Calibration Curve Dimensions	# points	range
5	GC-FID	DB-5MS	30m x 0.25 mm, 0.25µm film	6	0.5 - 20 ng/µL
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	6	0.1-10 ng/µL

Lab #	Instrument	**Alkanes and Alkenes** Phase	Dimensions	Calibration Curve # points	range
1a	GC/EI-MS	DB-17 MS	30m x 0.25 mm, 0.25µm film	5	1 - 50 ug/g
1c	GC/MS	DB-17	60m x 0.25 mm, 0.25µm film	5	0.03 - 66 ug/mL
4	GC/EI-MS	HP-5MS	30m x 0.25 mm, 0.25µm film	3	2.5 - 10 ng/µL
5	GC-FID	DB-5MS	30m x 0.25 mm, 0.25µm film	6	1.29 - 90.2 ng/µL
9	GC-TOFMS	Thermo TR-5MS	15m x 0.25 mm, 0.25µm film	5	0.5-150 ng/µL
10a	GC/MS	5% phenyl	30m x 0.25 mm, 0.25µm film	5	1-10
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	5	0.25-5 ng/µL
12	GC/MS	HP-5MS	60m x 0.25 mm, 0.25µm film	5	1-15 ng/µL

Lab #	**Hopanes, Cholestanes, Sterols** Instrument	Phase	Dimensions	Calibration Curve # points	range
1a	GC/MS	DB-17 MS	30m x 0.25 mm, 0.25µm film	5	100 - 5000 ng/g
5	GC-FID	DB-5MS	30m x 0.25 mm, 0.25µm film	6	0.5 - 20 ng/µL
10a	GC/MS	5% phenyl	30m x 0.25 mm, 0.25µm film	5	0.04-2
10b	GC/HRMS	5% phenyl	30m x 0.25 mm, 0.25µm film	5	0.0005-0.02
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	6	0.2-7 ng/µL
12	GC/MS	HP-5MS	60m x 0.25 mm, 0.25µm film	1	0.5 ng/µL

Lab #	Instrument	**Carbonyls and Acids** Phase	Dimensions	Calibration Curve # points	range
5	GC-FID	DB-5MS	30m x 0.25 mm, 0.25µm film	6	6 - 121 ng/µL
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	6	0.2-10 ng/µL
12	GC/MS	HP-5MS	60m x 0.25 mm, 0.25µm film	5	1-15 ng/µL

Lab #	Instrument	**Phenols** Phase	Dimensions	Calibration Curve # points	range
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	6	0.2-10 ng/µL

Lab #	Instrument	**Sugars** Phase	Dimensions	Calibration Curve # points	range
5	GC-FID	DB-5MS	30m x 0.25 mm, 0.25µm film	6	0.5 - 100 ng/µL
11	GC-ITD MS	VF-5	30m x 0.25 mm, 0.25µm film	6	0.2-10 ng/µL
12	GC/MS	HP-5MS	60m x 0.25 mm, 0.25µm film	3	6.16-61 ng/µL

Lab #	IS/surrogate added prior to extraction	Used?	PAHs added prior to analysis	Used?	corrected for recovery?
1a	deuterated naphthalene, biphenyl, acenaphthene, phenanthrene, fluoranthene, pyrene, B[a]A, B[a]P, perylene, B[ghi]P, DB[a,h]A	x			n
1b	deuterated naphthalene, biphenyl, acenaphthene, phenanthrene, fluoranthene, pyrene, B[a]A, B[a]P, perylene, B[ghi]P, DB[a,h]A	x			n
1c	deuterated naphthalene, biphenyl, acenaphthene, phenanthrene, fluoranthene, pyrene, B[a]A, B[a]P, perylene, B[ghi]P, DB[a,h]A	x			n
2	ES				
3a	ES				
3b	deuterated napthalene, biphenyl, phenanthrene, pyrene, B[a]A, B[a]P, B[ghi]P	x	deuterated anthracene		
4	deuterated fluorene, phenanthrene, anthracene, fluoranthene, pyrene, B[a]A, chrysene, B[b]F, B[k]F, B[e]P, B[a]P, perylene, B[ghi]P, I[1,2,3-cd]P, DB[a,h]A	x			
6	deuterated naphthalene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, chrysene, B[k]F, B[e]P, B[a]P, perylene, indeno(1,2,3-cd)pyrene, B[ghi]P		deuterated acenaphthylene, B[a]A, B[b]F	x	y
7	see notes (Appendix B)		deuterated fluoranthene	x	
8	SRM 2270 - Perdeuterated PAH II Solution	x			
9	ES				
11	deuterated naphthalene, biphenyl, acenaphthene, phenanthrene, anthracene, pyrene, B[a]A, chrysene, B[e]P, B[a]P, perylene, B[ghi]P, coronene	x			
12	deuterated acenaphthylene, eicosane, chrysene, DB[a,h]A				
14	ES				

Lab #	IS/surrogate added prior to extraction	Used?	Nitro-PAHs added prior to analysis	Used?	corrected for recovery?
1a	deuterated 1-nitorpyrene, 3-nitrofluoranthene, 9-nitroanthracene, and 6-nitrochrysene	x			n
4	deuterated 9-nitroanthracene, 1-nitropyrene, 6-nitrochrysene, 6-nitroB[a]P	x			
7	see notes (Appendix B)	x	deuterated 2-nitrodibenzodioxin, 7-nitroB[a]A		

Lab #	IS/surrogate added prior to extraction	Used?	PAH-quinones added prior to analysis	Used?	corrected for recovery?
5			deuterated tetracosane	x	
11	same as PAHs	x			

Lab #	IS/surrogate added prior to extraction	Used?	**Alkanes and Alkenes** added prior to analysis	Used?	corrected for recovery?
1a	deuterated n-dodecane, n-eicosane, n-triacontane	x			n
1c	deuterated n-dodecane, n-eicosane, n-triacontane	x			n
4	deuterated C20, C24, C30	x			
5	deuterated tetracosane	x			
9	ES				
10	mixture of Deuterated C12, C16, 20, C24, C30, C32, C36	x	1-phenyldodecane	x	y
11	deuterated didecabe, hexadecane, eicosane, tetracosane, octacosane, triacontane	x			
12	deuterated dodecane, hexadecane, eicosane, octacosane, hexatriacontane				

Lab #	IS/surrogate added prior to extraction	Used?	**Hopanes, Cholestanes, Sterols** added prior to analysis	Used?	corrected for recovery?
1a	deuterated n-dodecane, n-eicosane, n-triacontane	x			n
5	C18-d acid	x			
10	B,B-hopane	x	5α-androstane	x	y
11	deuterated cholesterol	x			
12	deuterated -aaa-20R-cholestane				

Lab #	IS/surrogate added prior to extraction	Used?	**Carbonyls and Acids** added prior to analysis	Used?	corrected for recovery?
5	C18-d acid	x			
11	deuterated hexanoic acid, benzoic acid, succinic acid, adipic acid, suberic acid, homovanillic acid, myristic acid, oleic acid, tetradecanedioic acid, eicosanoic acid	x			
12	deuterated decanoic acid, heptadecanoic ackd				

Lab #	IS/surrogate added prior to extraction	Used?	**Phenols** added prior to analysis	Used?	corrected for recovery?
11	deuterated benzoic acid	x			

Lab #	IS/surrogate added prior to extraction	Used?	**Sugars** added prior to analysis	Used?	corrected for recovery?
5	C18-d acid	x			
11	carbon-13 labeled levoglucosan	x			
12	carbon-13 labeled levoglucosan				

Appendix D

Charts of SRM 1648, Baltimore-2 PM, and Filter Samples (RM 8785) along with SRM 1649a: Results by Analyte

See Tables 1 through 4 for results reported as *<number*, detection limit, etc. Charts for analytes with only one reported numerical result are not included in this appendix.

For SRM 1648, Baltimore-2 PM, and RM 8785 plots:

Solid line: exercise assigned value

Dotted line: $z = \pm 1$, i. e., 25 % from assigned value

Dotted/dashed line: $z = \pm 2$, i. e., 50 % from assigned value

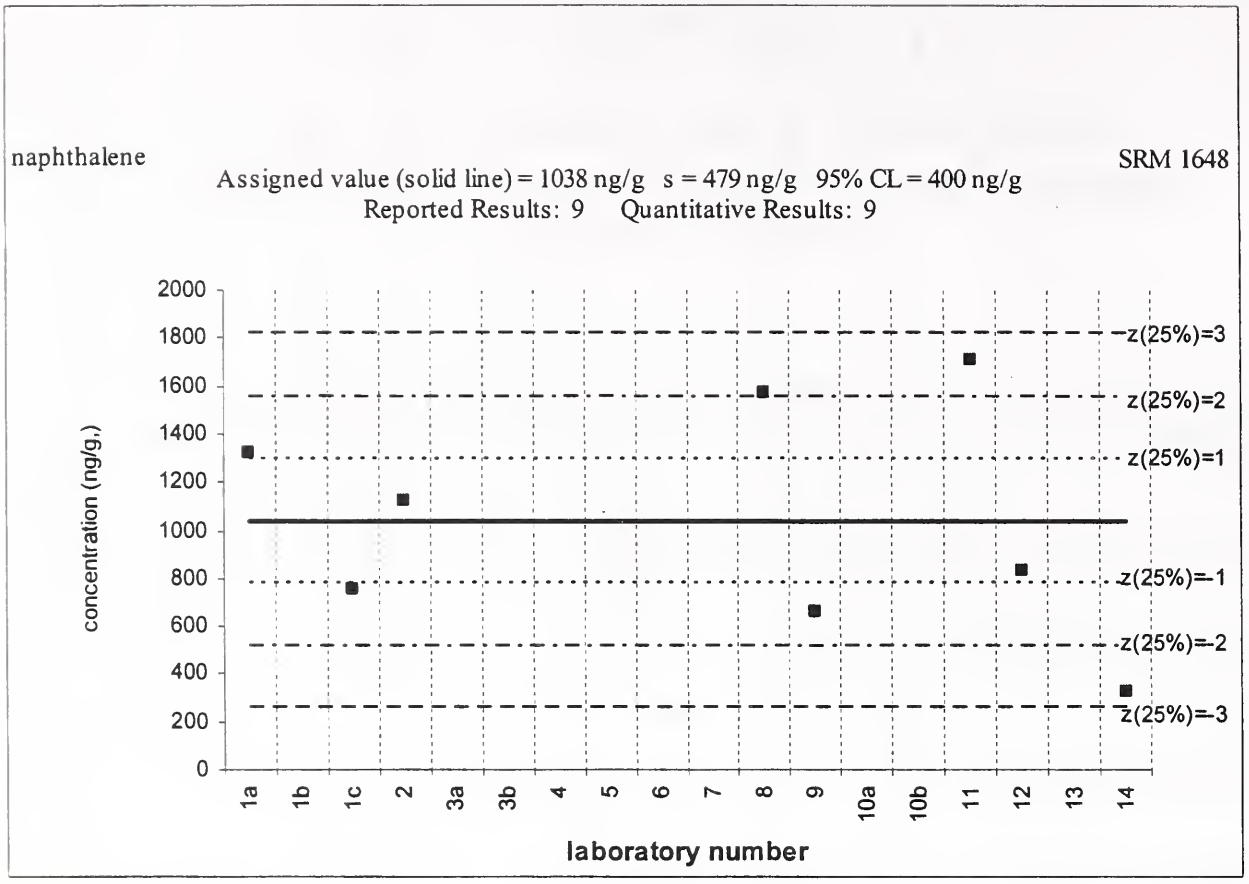
Dashed line: $z = \pm 3$, i. e., 75 % from assigned value

For SRM 1649a plots:

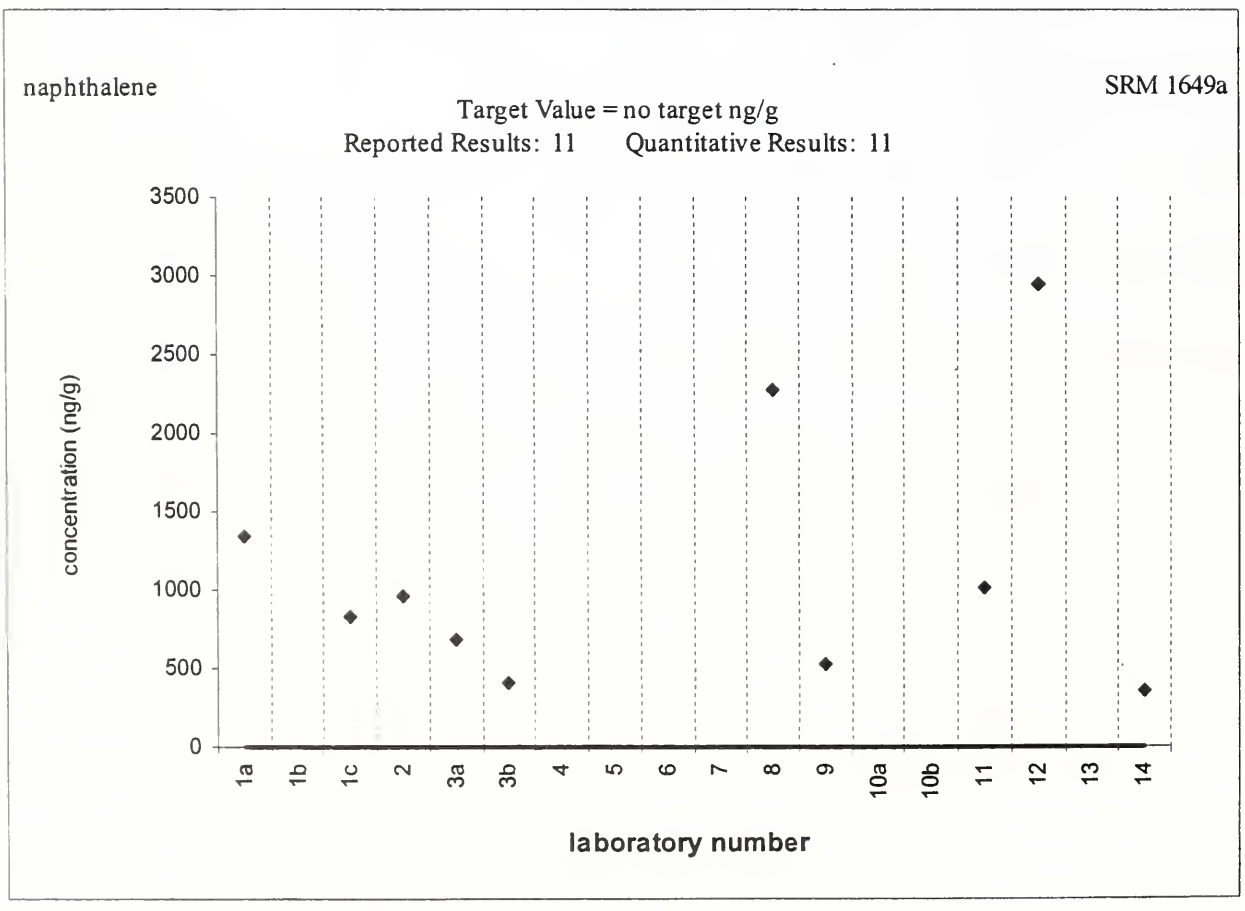
Solid line: material certified concentration or target value (see caption of each plot)

Dotted line: 95 % confidence interval (CI)

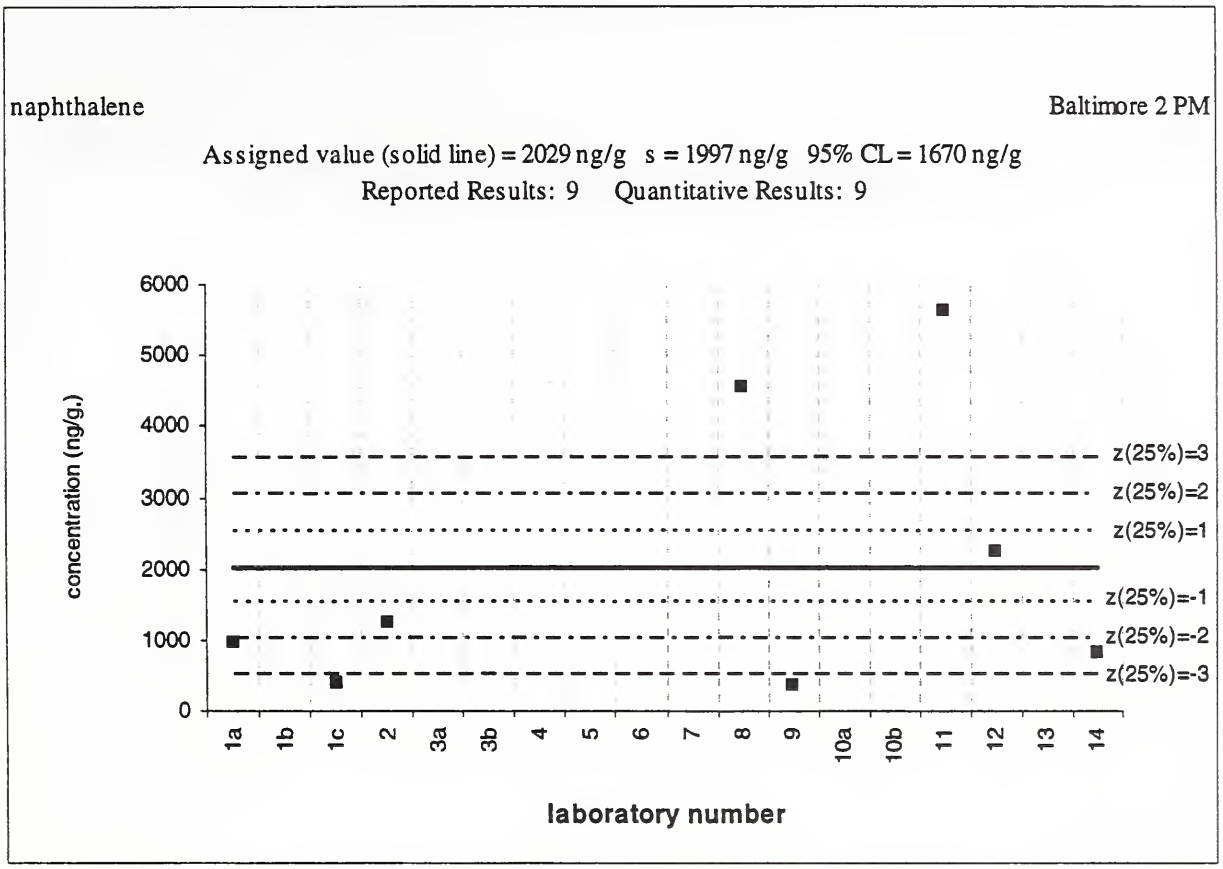
Dashed line: 30 % from 95 % confidence interval (CI)



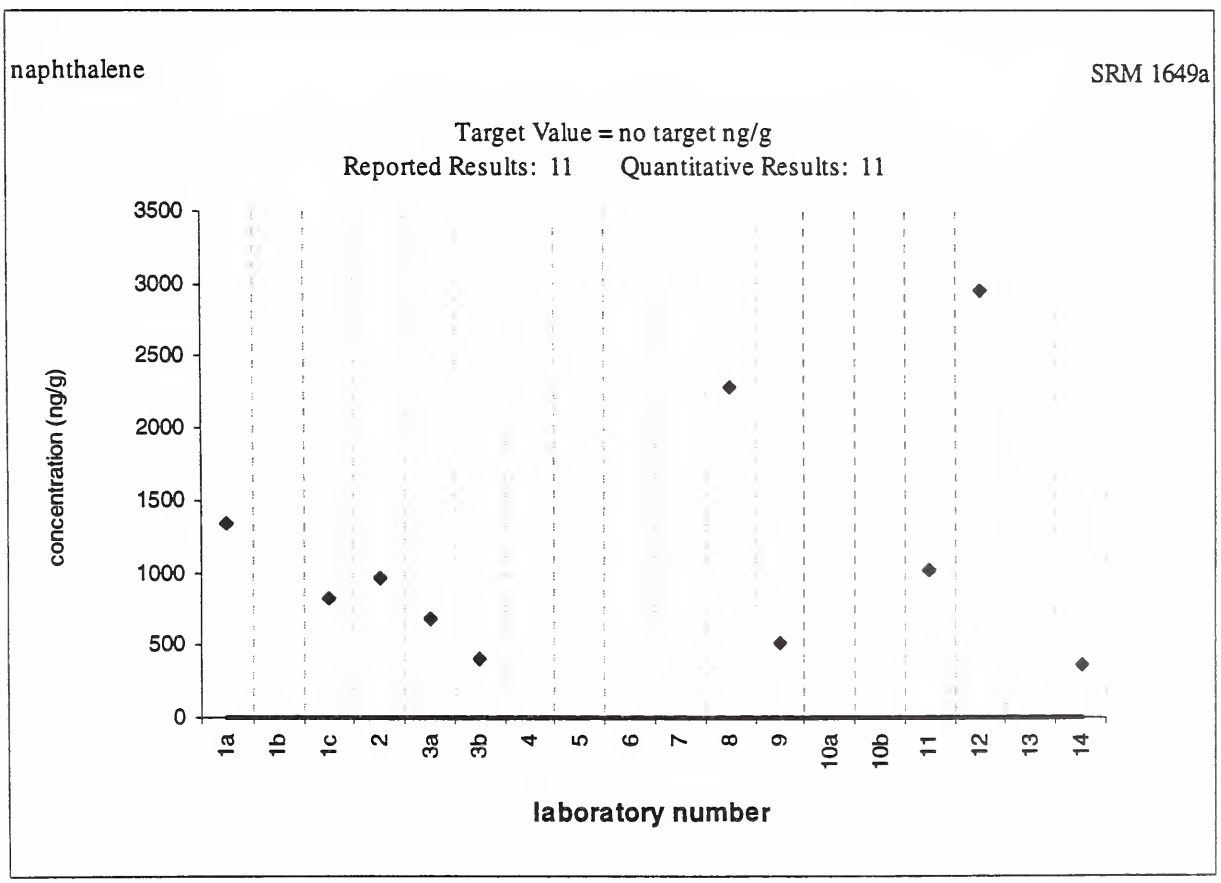
Lab 7 = 15716 ng/g



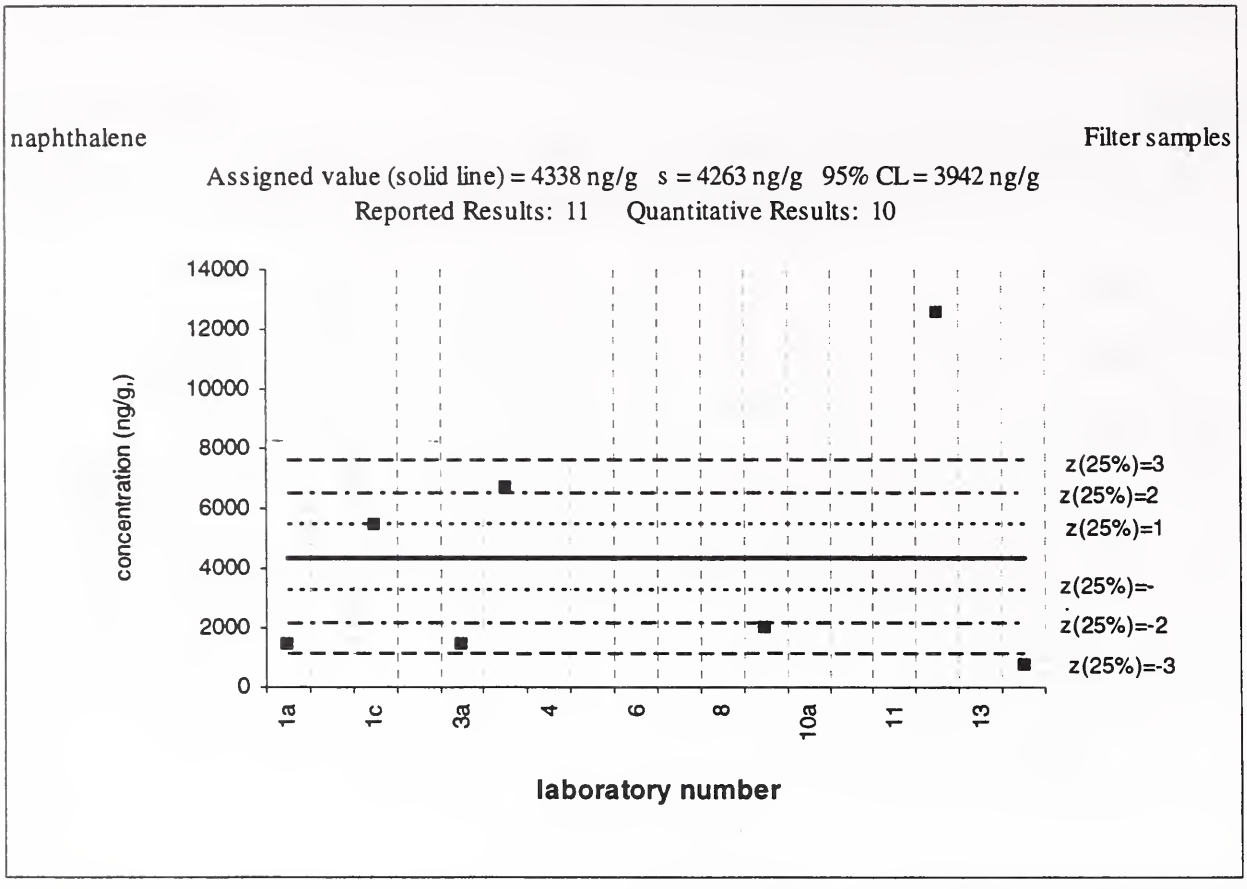
Lab 7 = 27984 ng/g



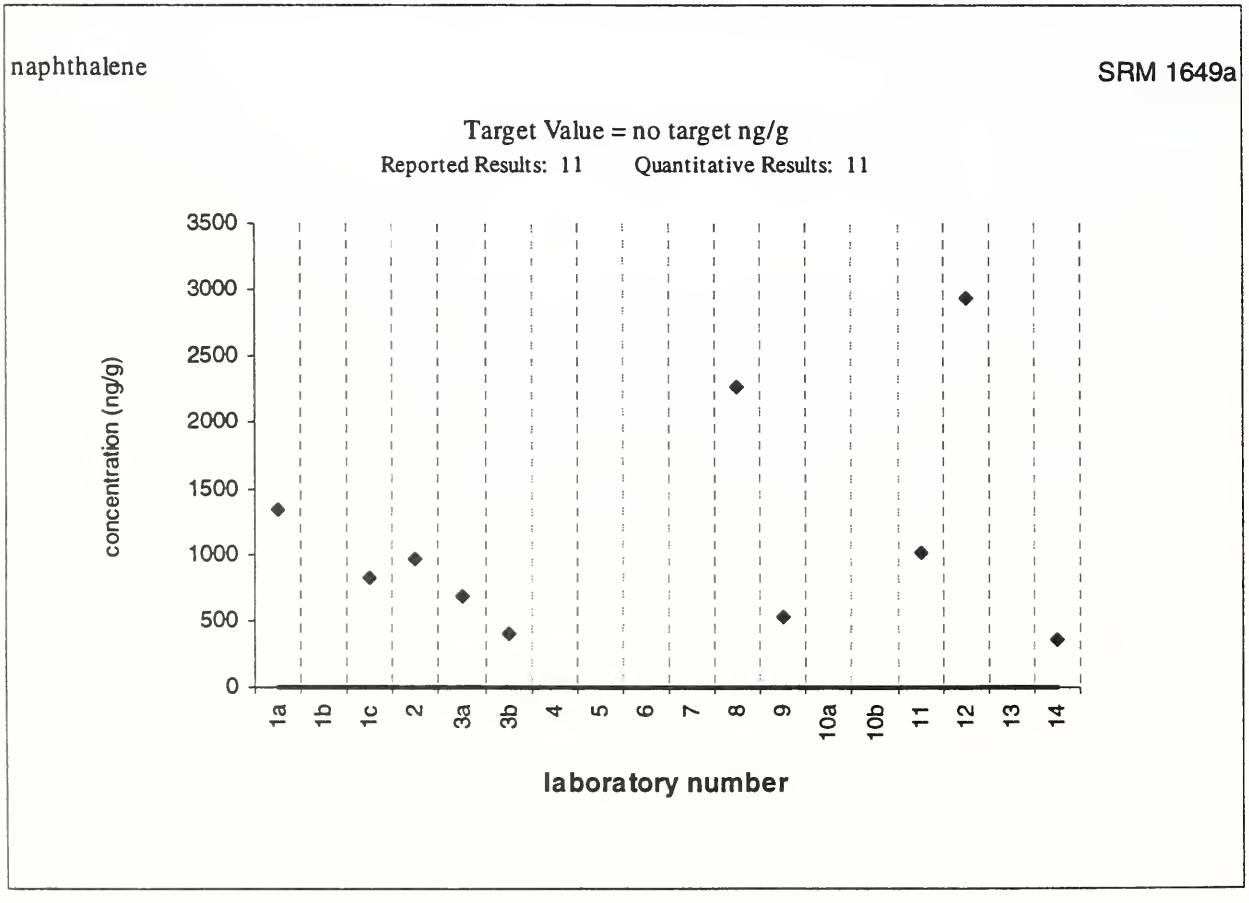
Lab 7 = 66090 ng/g



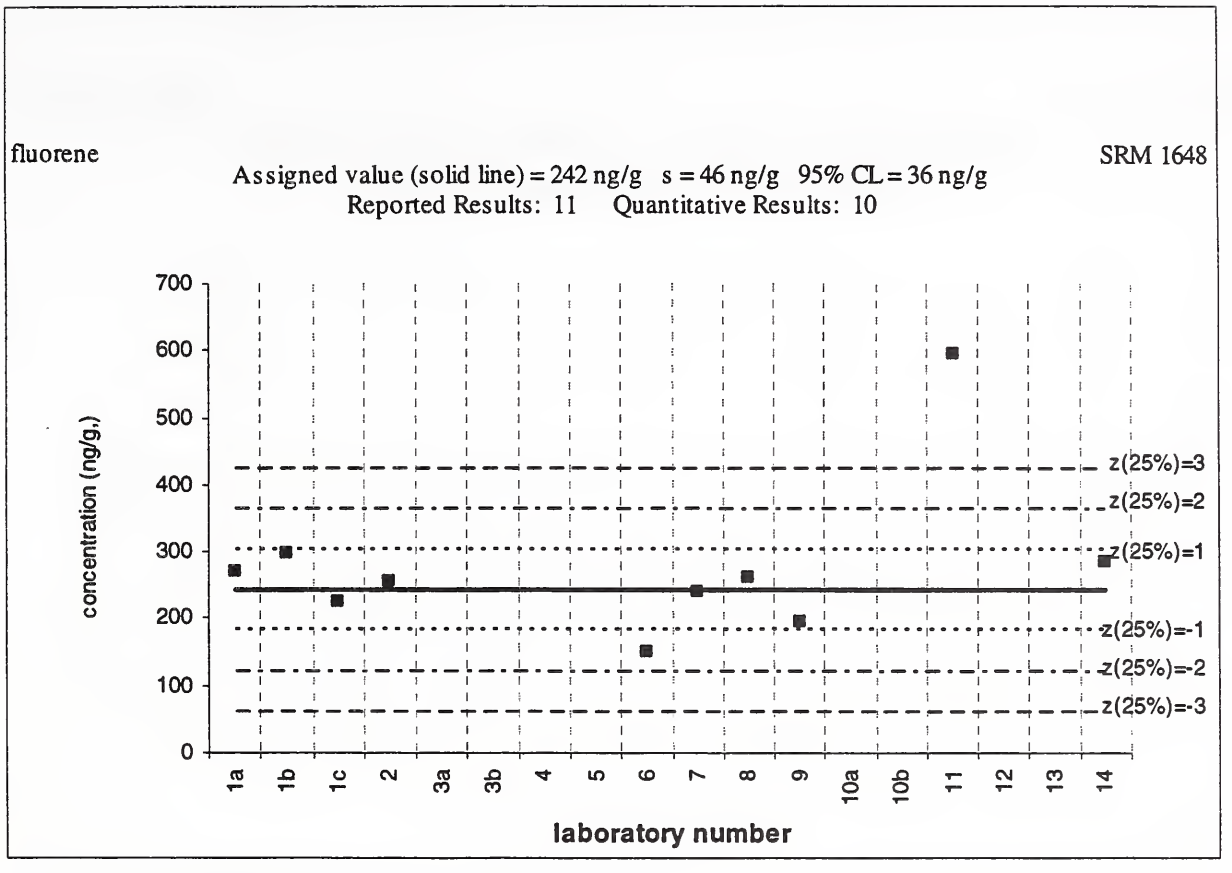
Lab 7 = 27984 ng/g

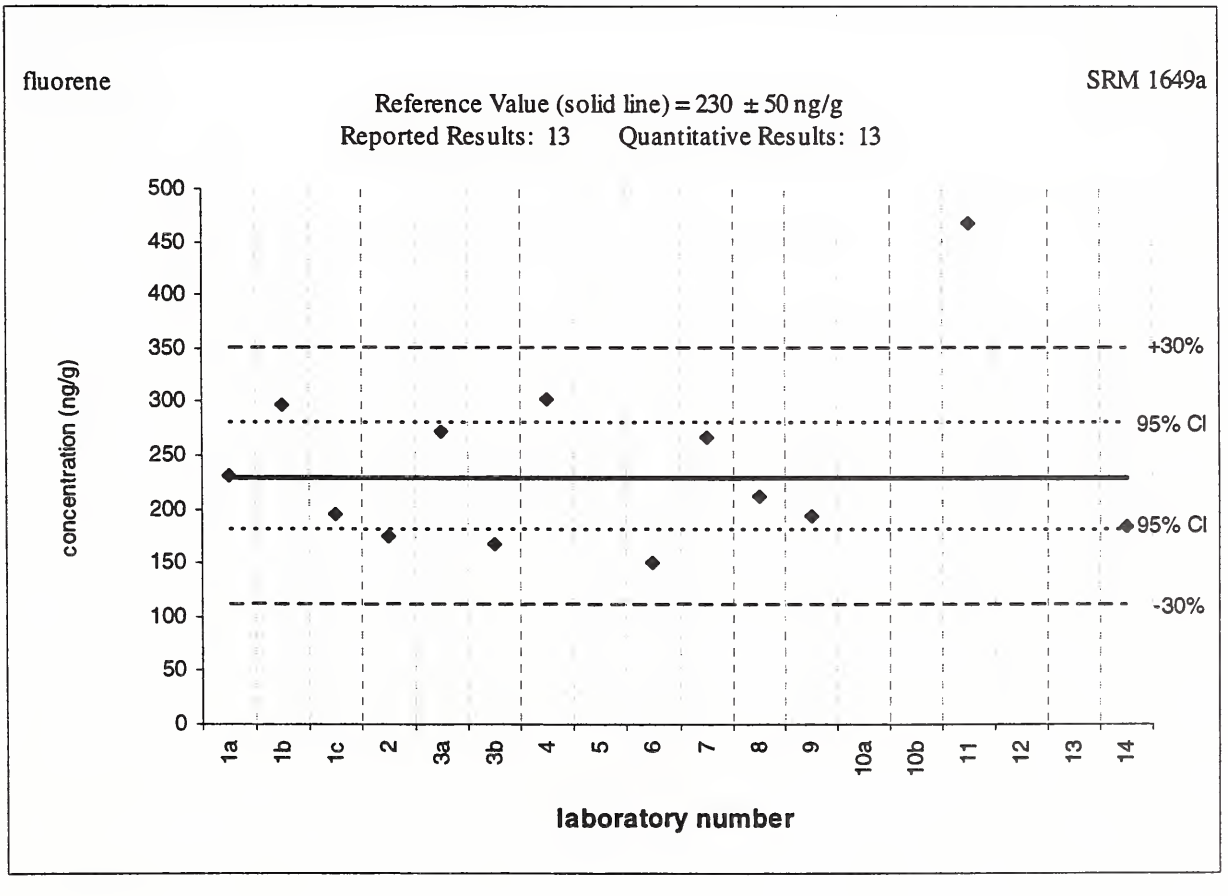


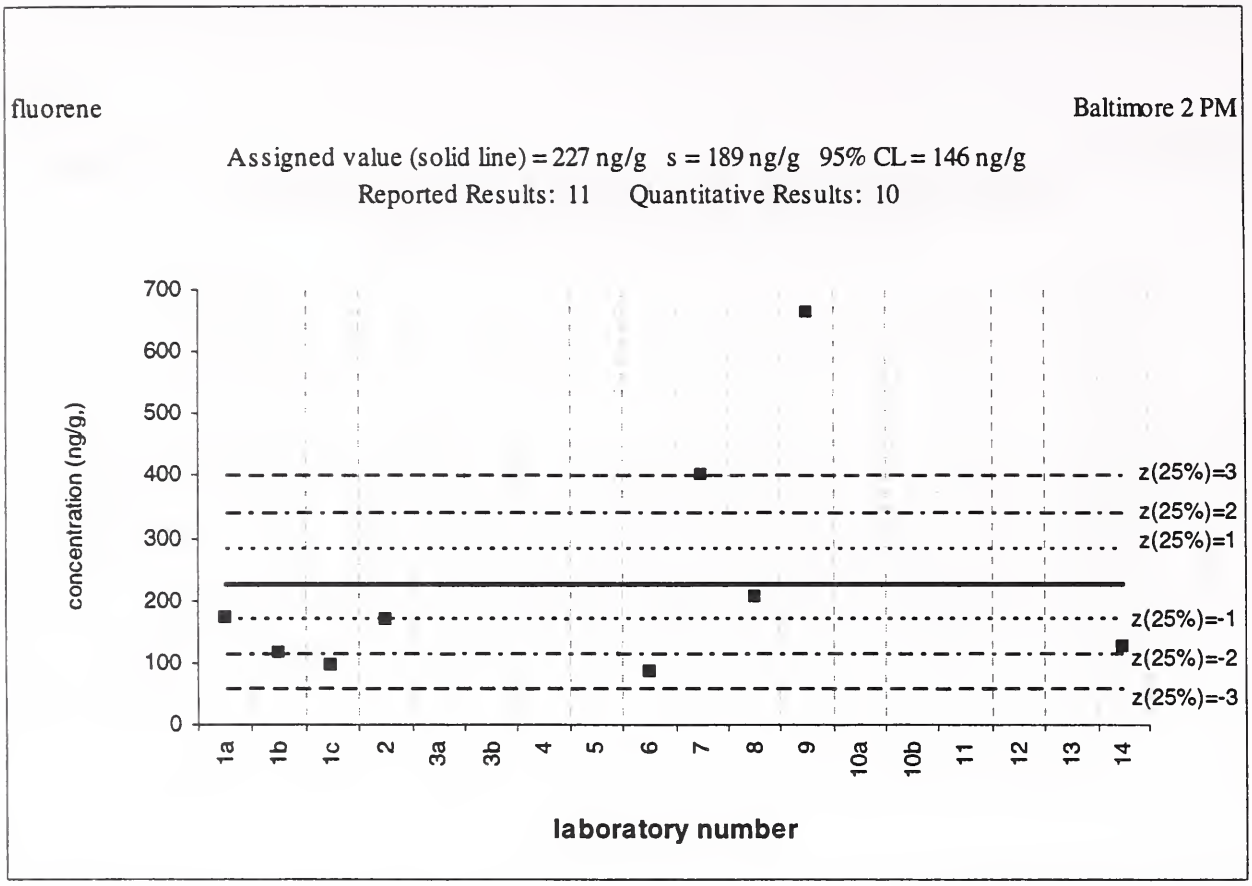
Lab 2 = 47213 ng/g; Lab 7 = 27984 ng/g; Lab 11 = 240250 ng/g



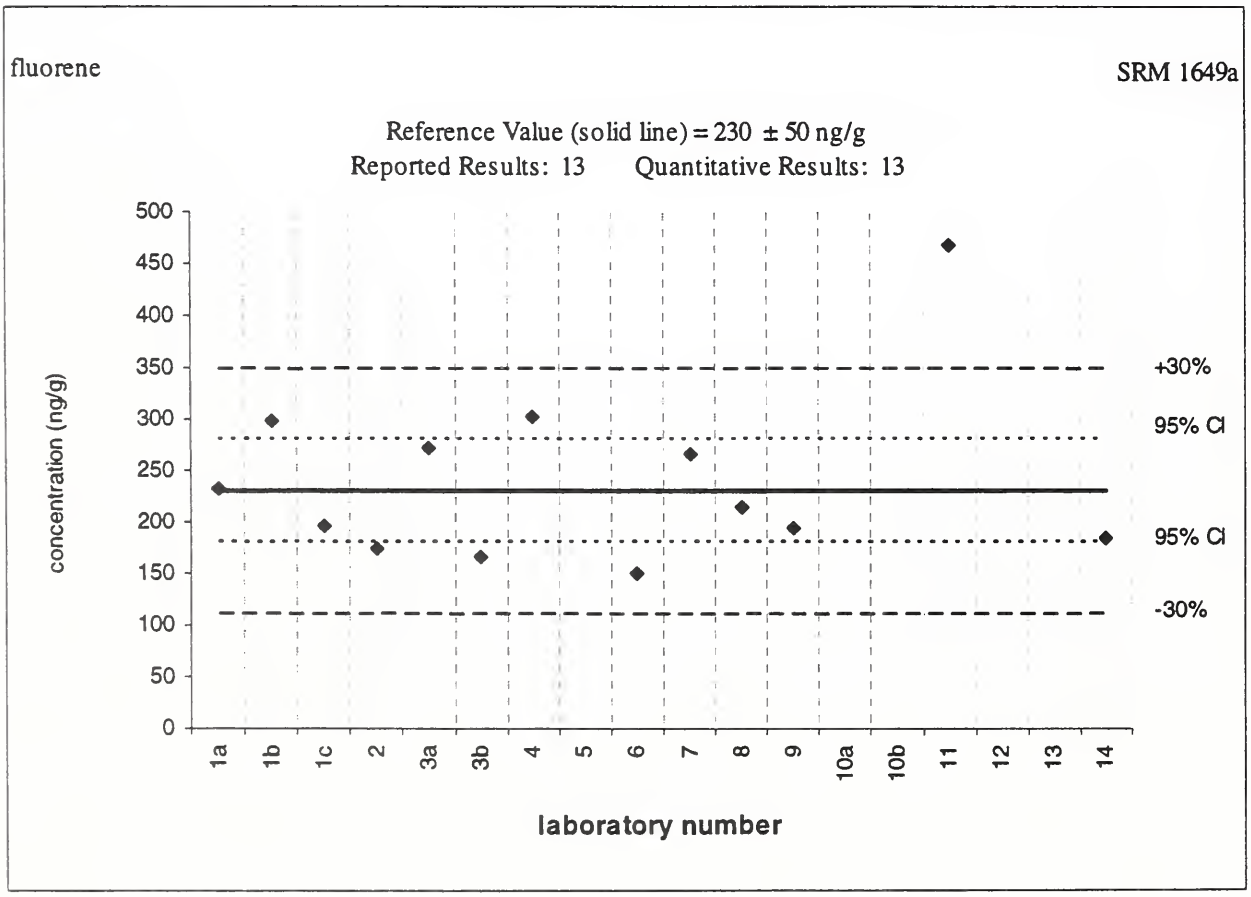
Lab 7 = 27984 ng/g


fluorene
SRM 1648
Assigned value (solid line) = 242 ng/g s = 46 ng/g 95% CL = 36 ng/g
Reported Results: 11 Quantitative Results: 10
concentration (ng/g)
700
600
500
400
300
200
100
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number


fluorene
SRM 1649a
Reference Value (solid line) = 230 ± 50 ng/g
Reported Results: 13 Quantitative Results: 13
concentration (ng/g)
500
450
400
350
300
250
200
150
100
50
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number



Lab 11 = 1646 ng/g

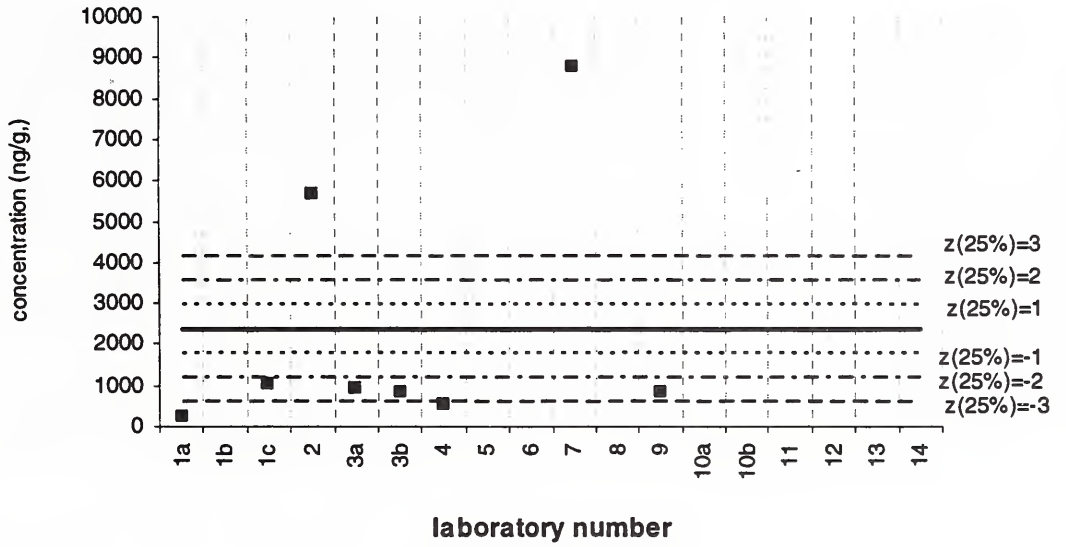


fluorene

Filter samples

Assigned value (solid line) = 4338 ng/g s = 4263 ng/g 95% CL = 3942 ng/g

Reported Results: 12 Quantitative Results: 9

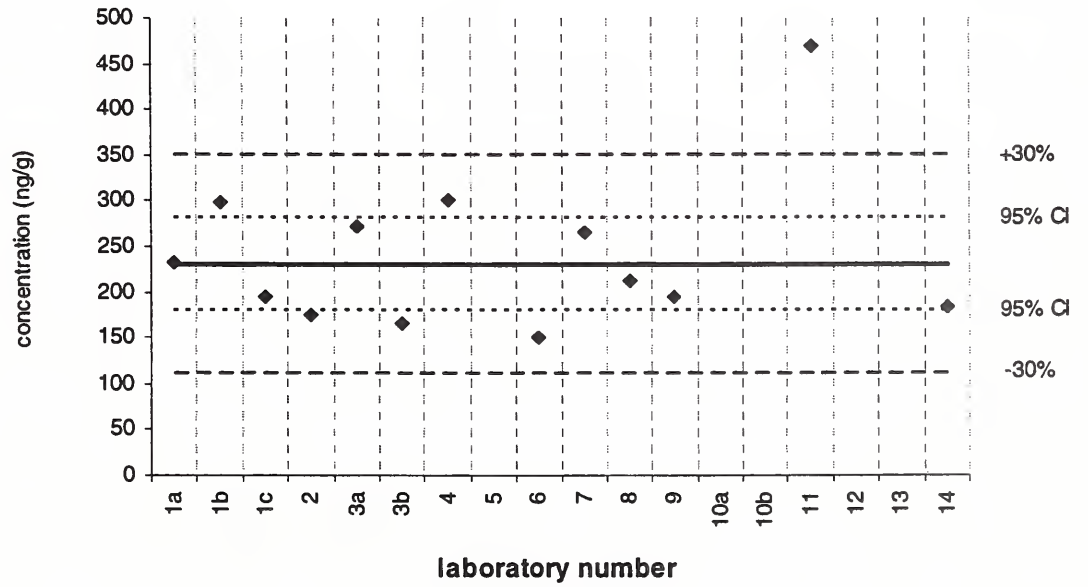


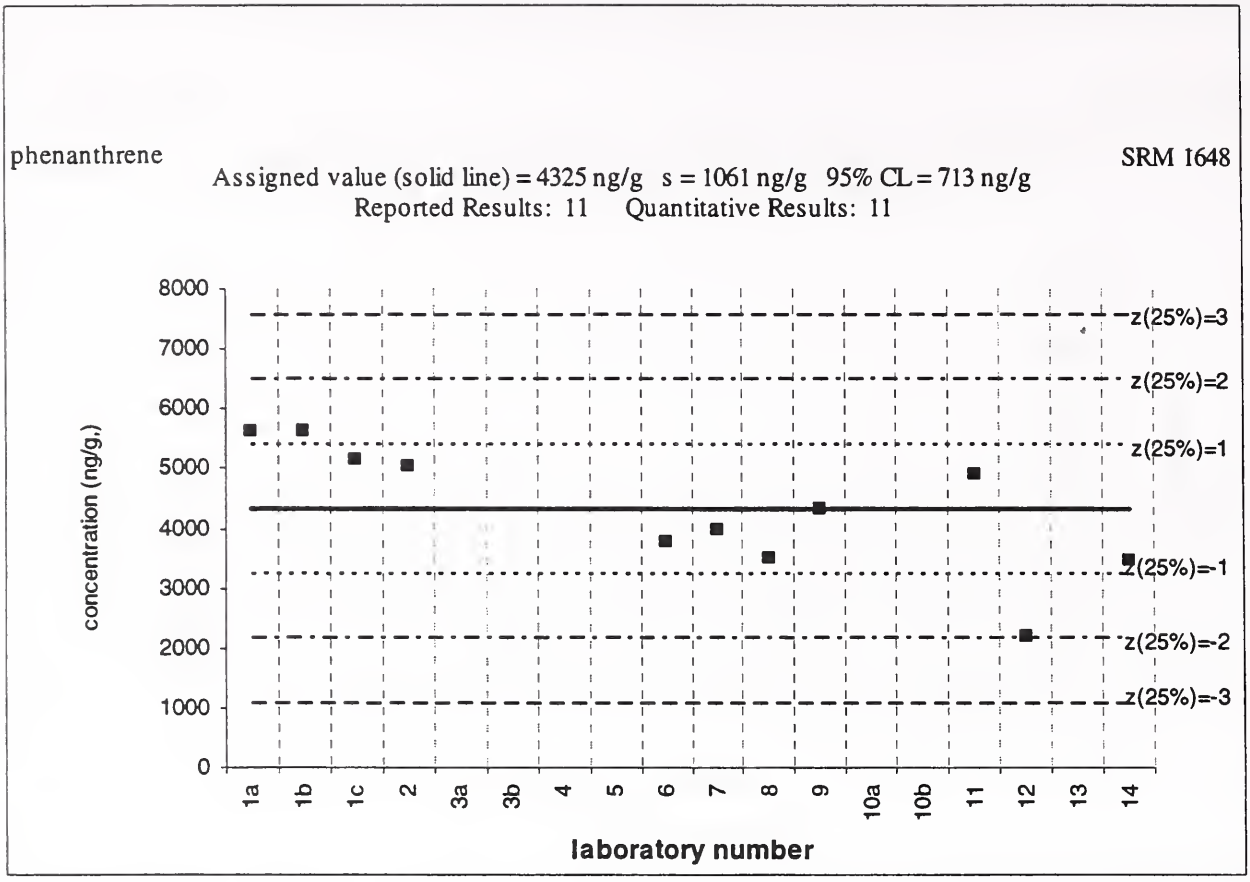
fluorene

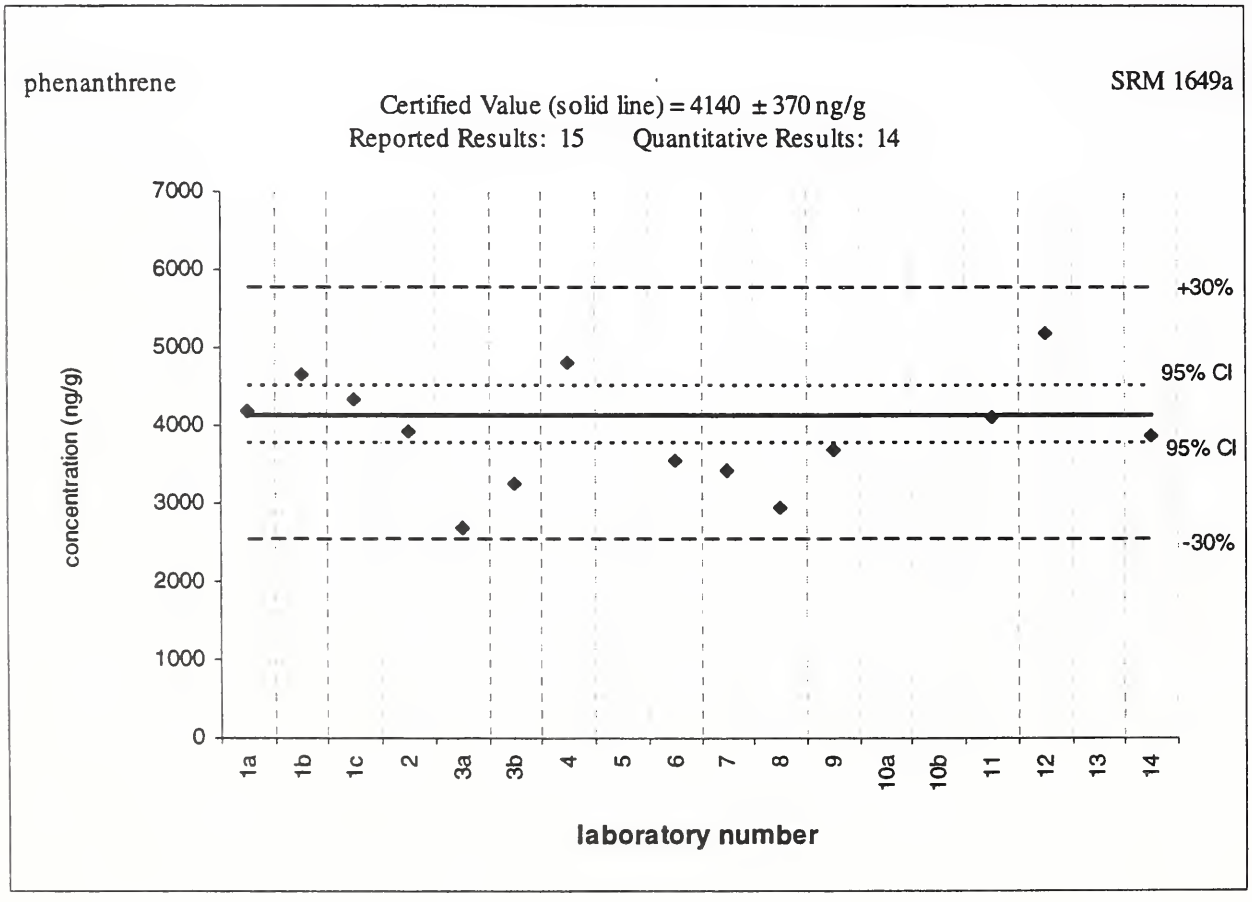
SRM 1649a

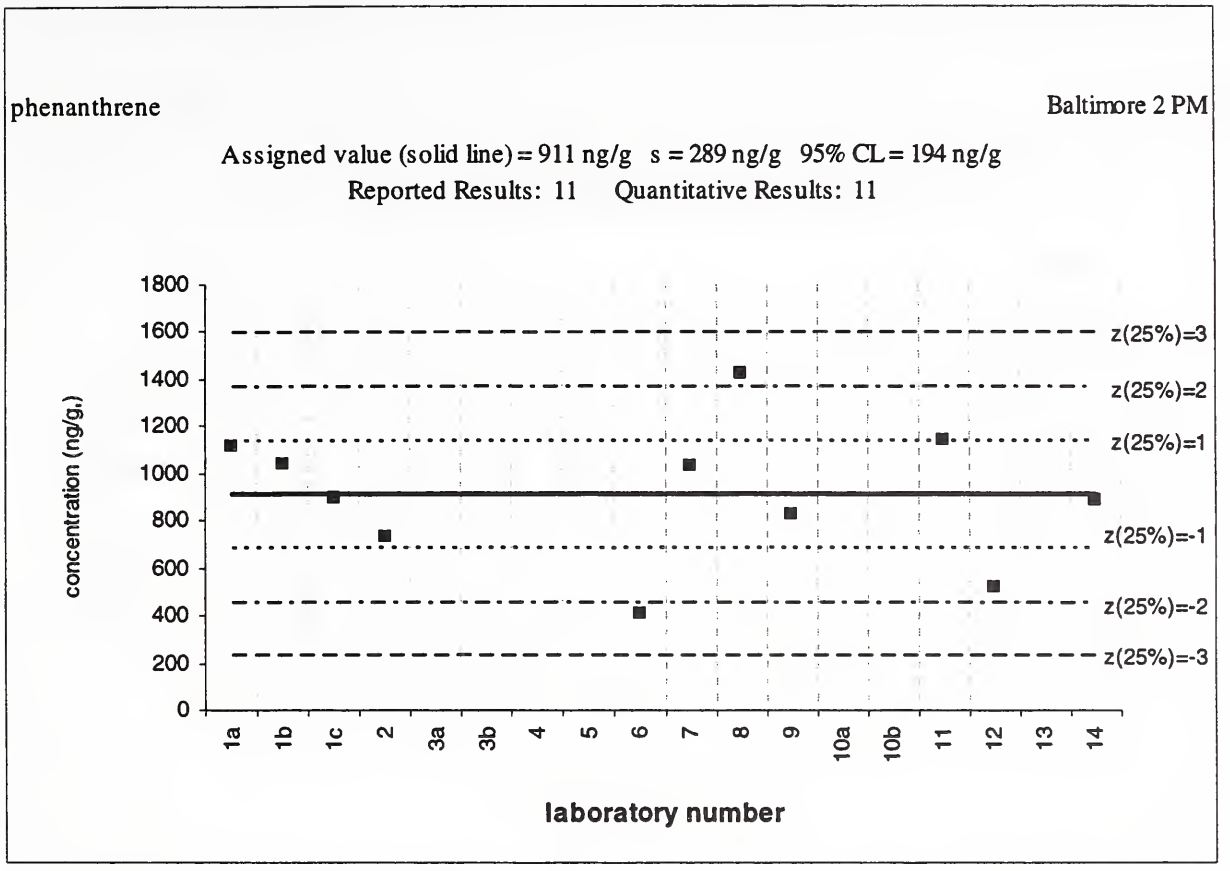
Reference Value (solid line) = 230 ± 50 ng/g

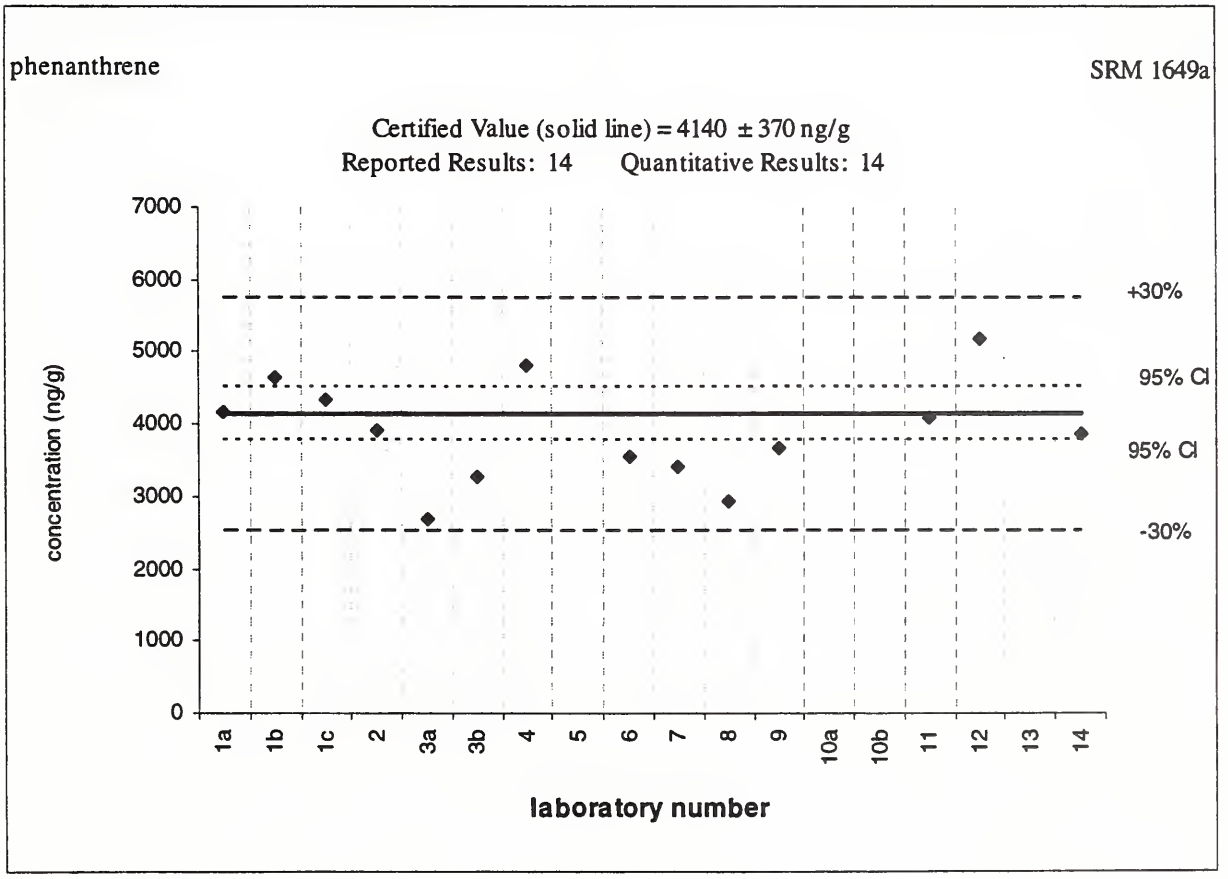
Reported Results: 13 Quantitative Results: 13




phenanthrene
SRM 1648
Assigned value (solid line) = 4325 ng/g s = 1061 ng/g 95% CL = 713 ng/g
Reported Results: 11 Quantitative Results: 11
concentration (ng/g)
8000
7000
6000
5000
4000
3000
2000
1000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number


phenanthrene
SRM 1649a
Certified Value (solid line) = 4140 ± 370 ng/g
Reported Results: 15 Quantitative Results: 14
concentration (ng/g)
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number


phenanthrene
Baltimore 2 PM
Assigned value (solid line) = 911 ng/g s = 289 ng/g 95% CL = 194 ng/g
Reported Results: 11 Quantitative Results: 11
concentration (ng/g)
1800
1600
1400
1200
1000
800
600
400
200
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

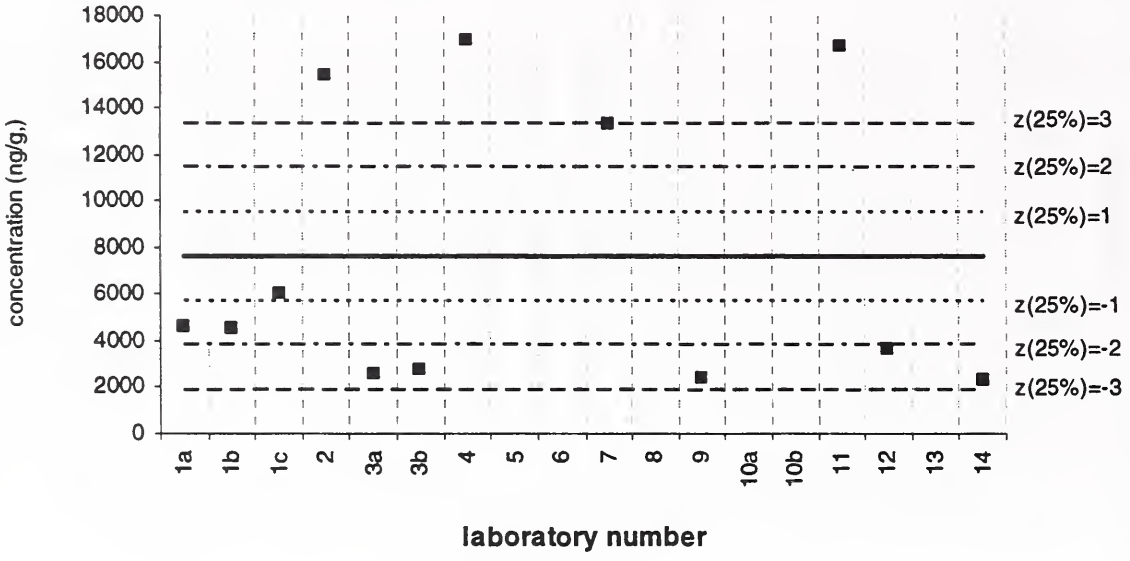

phenanthrene
SRM 1649a
Certified Value (solid line) = 4140 ± 370 ng/g
Reported Results: 14 Quantitative Results: 14
concentration (ng/g)
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

phenanthrene

Filter samples

Assigned value (solid line) = 7600 ng/g s = 6061 ng/g 95% CL = 3851 ng/g

Reported Results: 13 Quantitative Results: 12

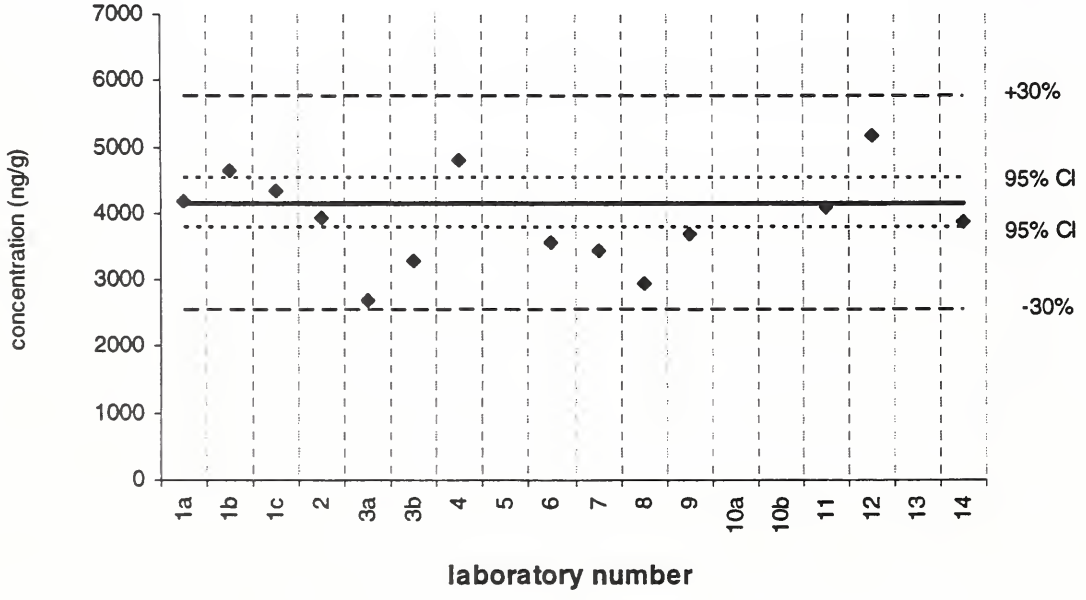


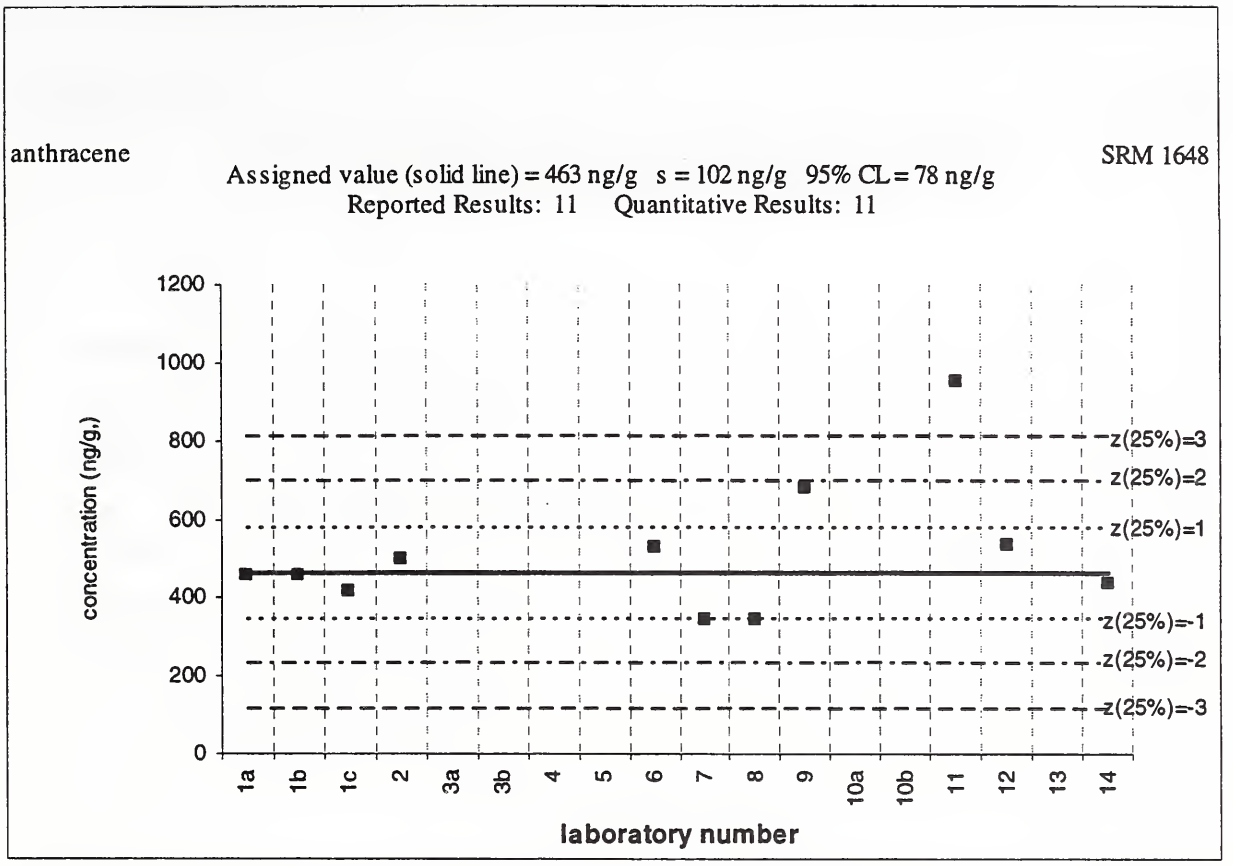
phenanthrene

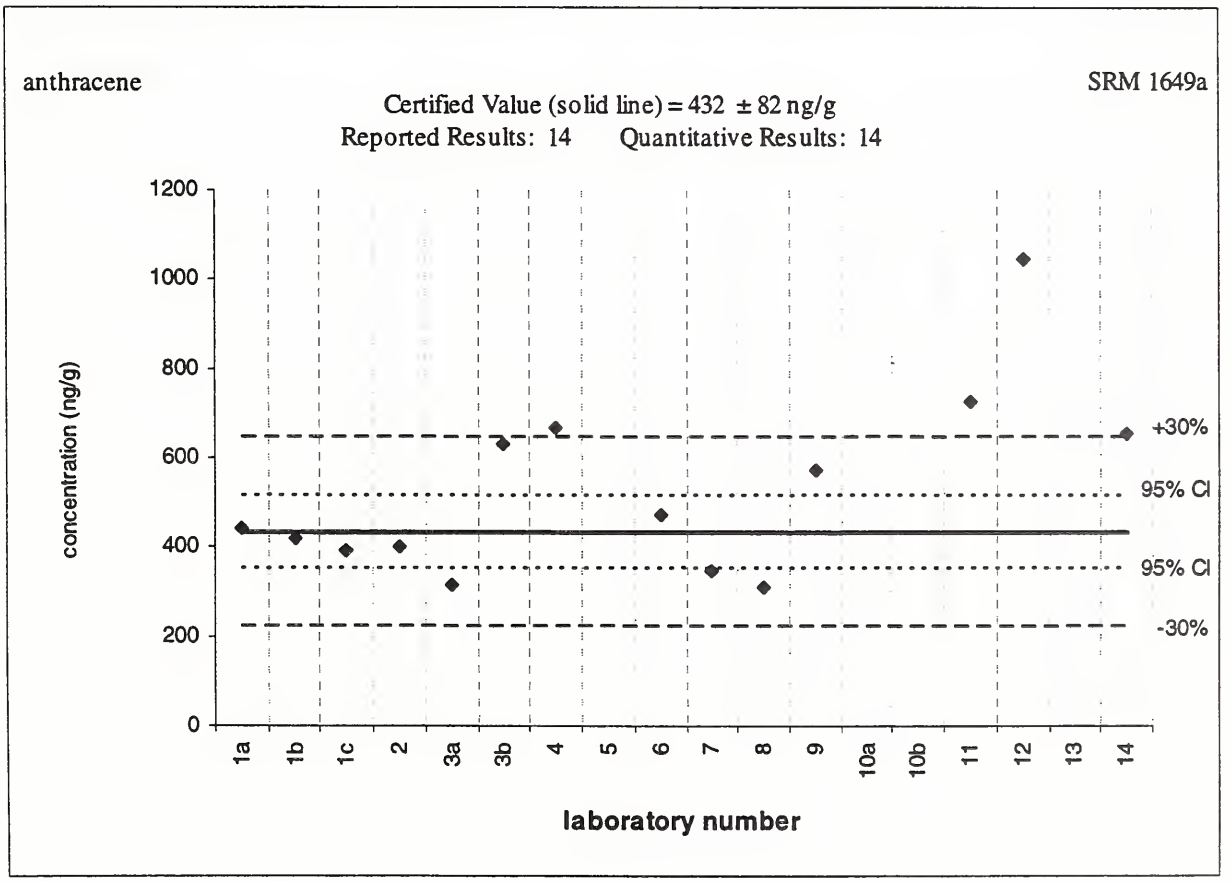
SRM 1649a

Certified Value (solid line) = 4140 ± 370 ng/g

Reported Results: 14 Quantitative Results: 14




anthracene
SRM 1648
Assigned value (solid line) = 463 ng/g s = 102 ng/g 95% CL = 78 ng/g
Reported Results: 11 Quantitative Results: 11
concentration (ng/g,)
1200
1000
800
600
400
200
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

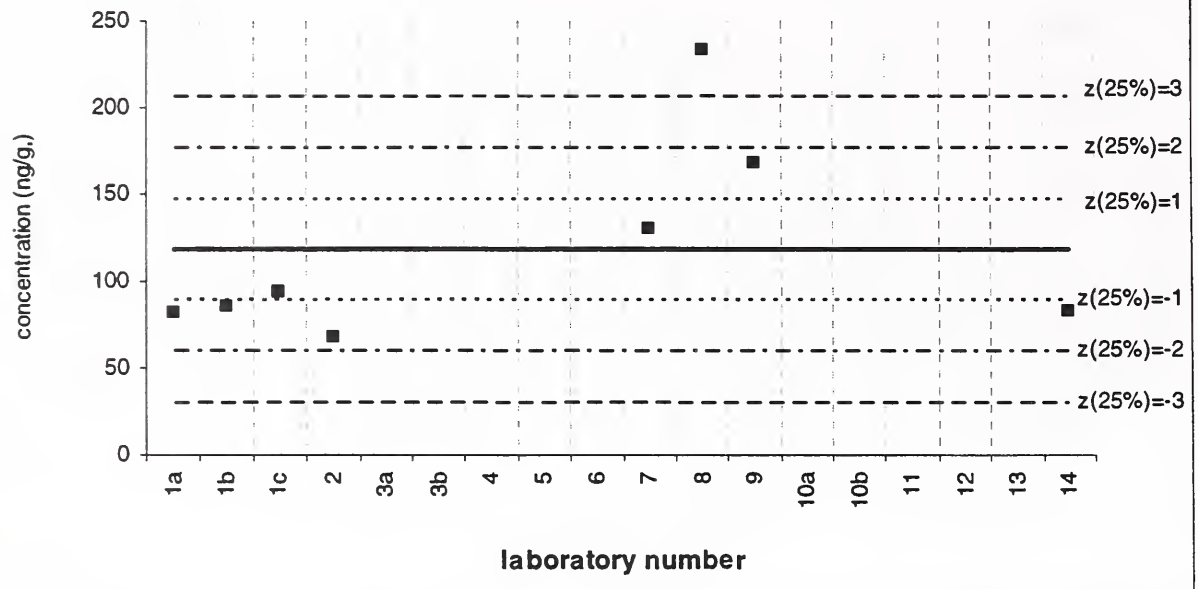

anthracene
SRM 1649a
Certified Value (solid line) = 432 ± 82 ng/g
Reported Results: 14 Quantitative Results: 14
concentration (ng/g)
1200
1000
800
600
400
200
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

anthracene

Baltimore 2 PM

Assigned value (solid line) = 118 ng/g s = 57 ng/g 95% CL = 48 ng/g

Reported Results: 11 Quantitative Results: 8

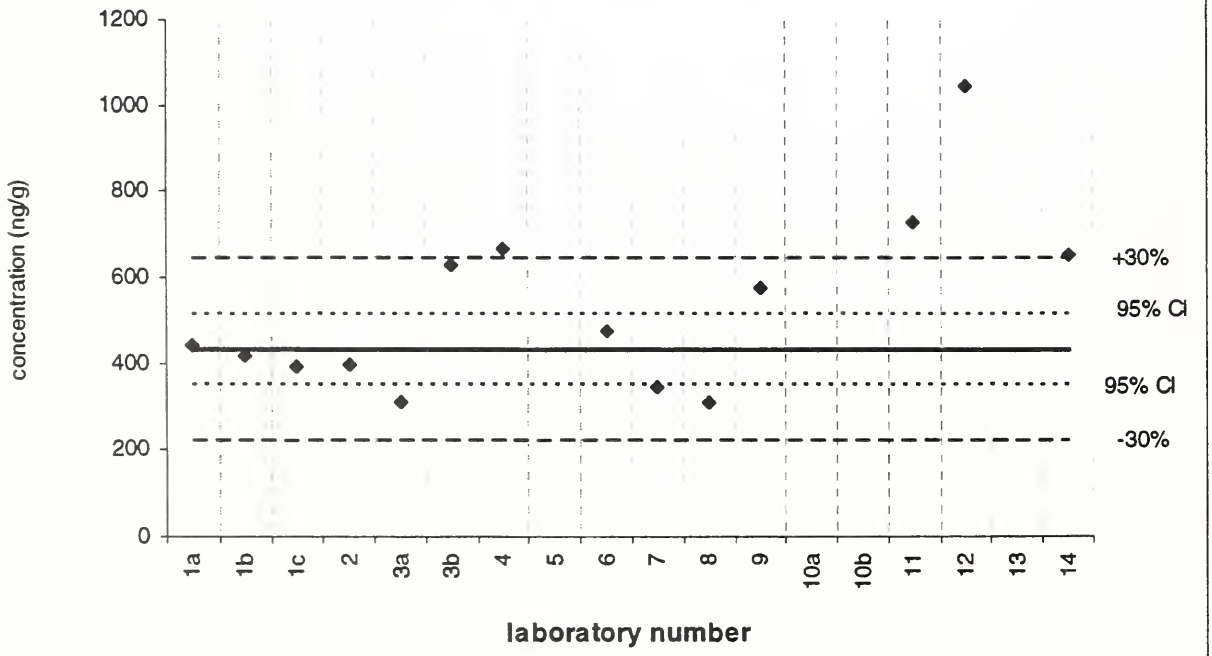


anthracene

SRM 1649a

Certified Value (solid line) = 432 ± 82 ng/g

Reported Results: 14 Quantitative Results: 14

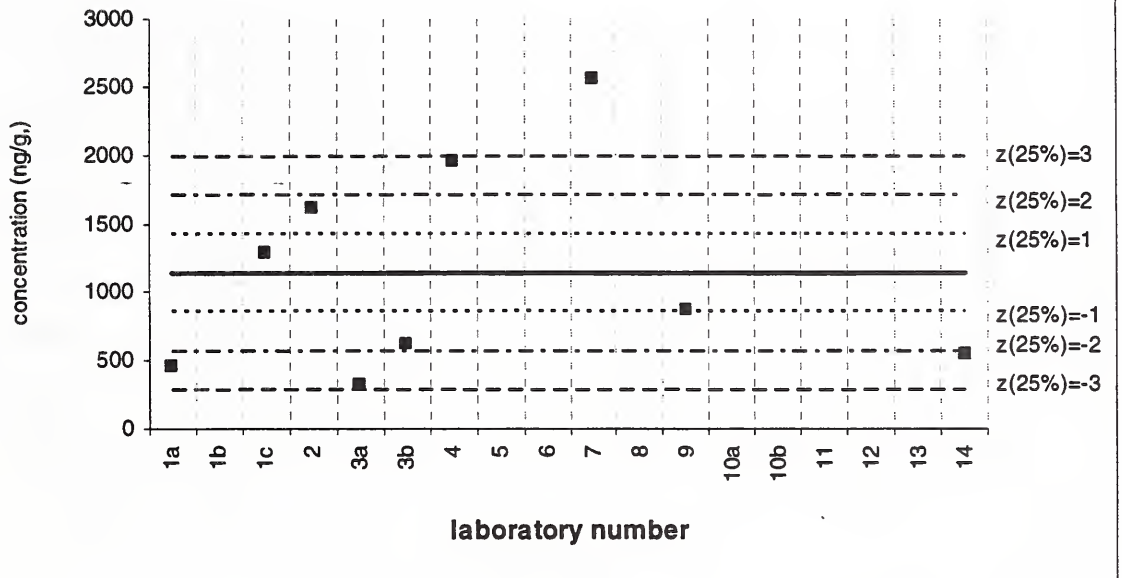


anthracene

Filter samples

Assigned value (solid line) = 1134 ng/g s = 766 ng/g 95% CL = 589 ng/g

Reported Results: 12 Quantitative Results: 9

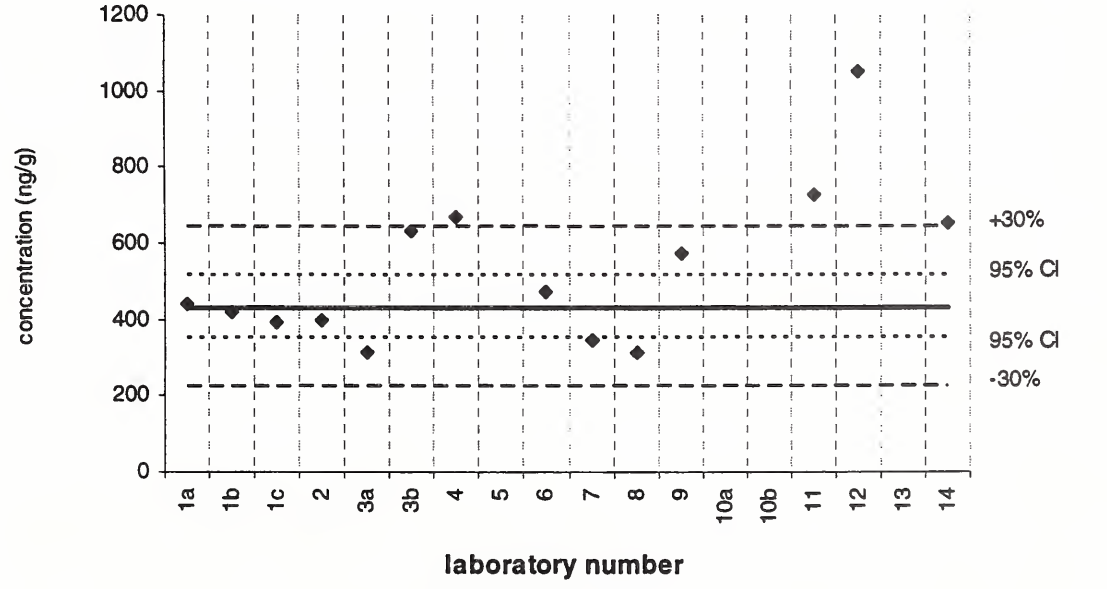


anthracene

SRM 1649a

Certified Value (solid line) = 432 ± 82 ng/g

Reported Results: 14 Quantitative Results: 14

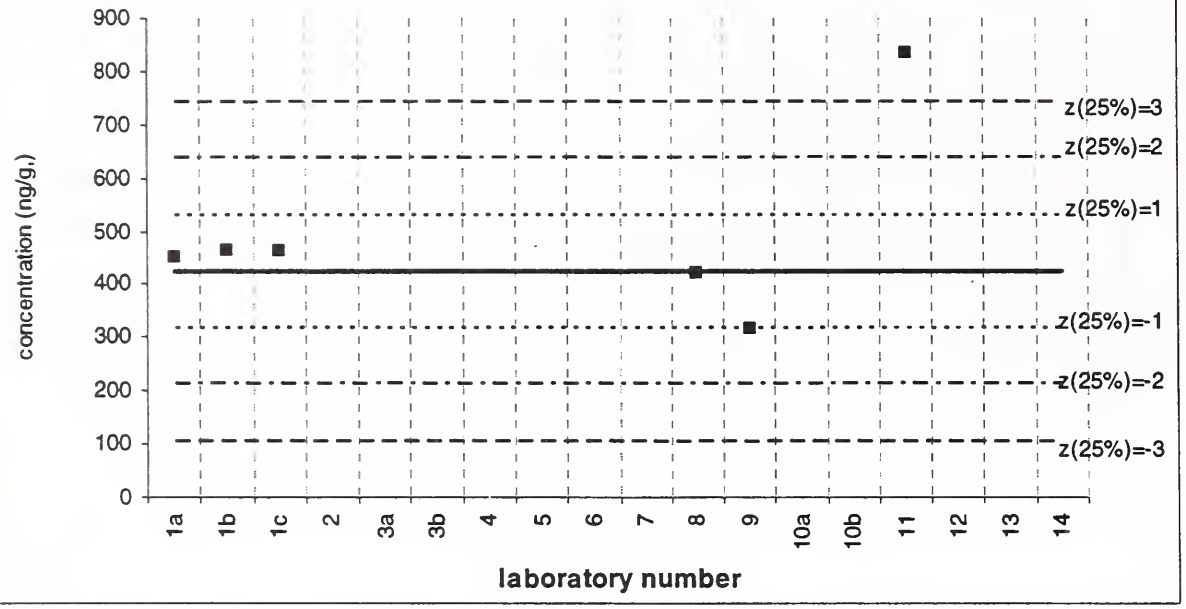


1-methylphenanthrene

SRM 1648

Assigned value (solid line) = 424 ng/g s = 62 ng/g 95% CL = 77 ng/g

Reported Results: 7 Quantitative Results: 6

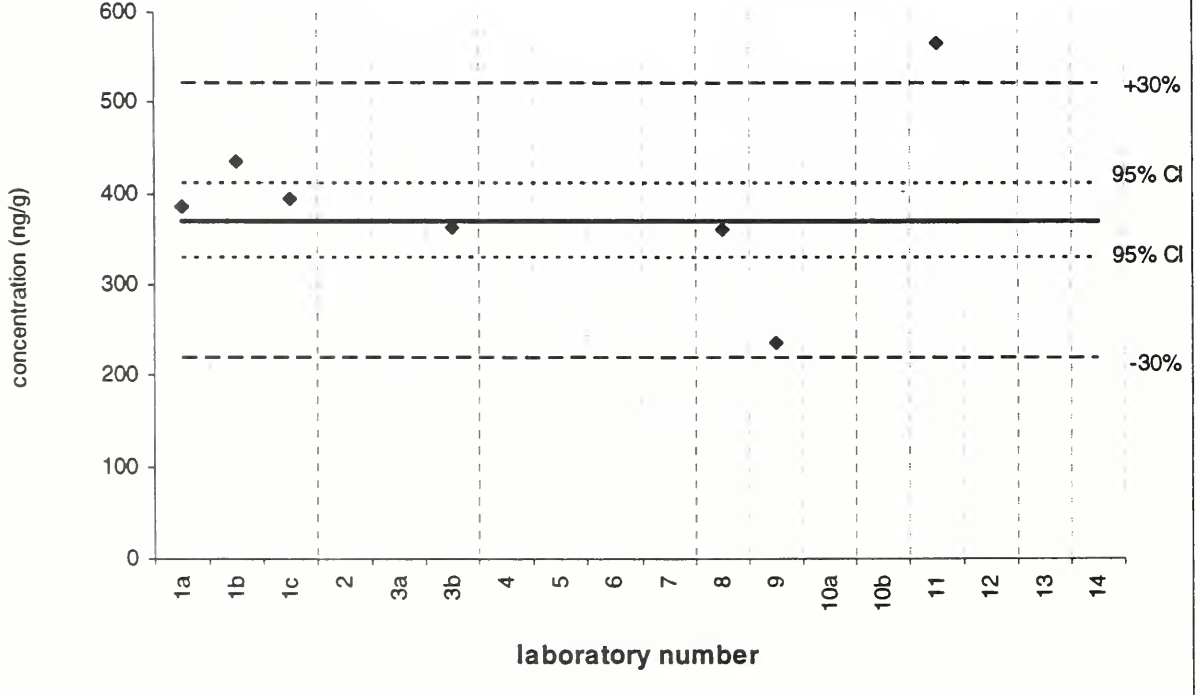


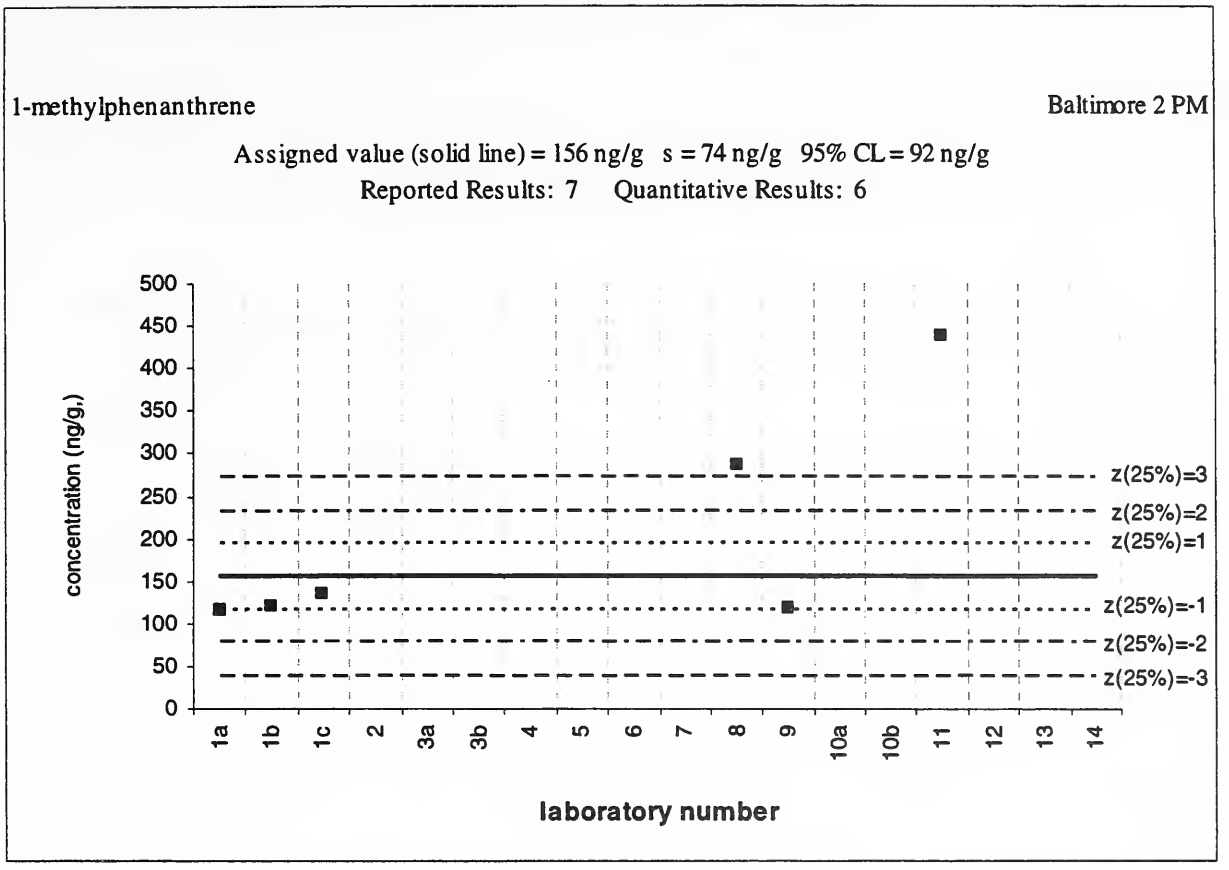
1-methylphenanthrene

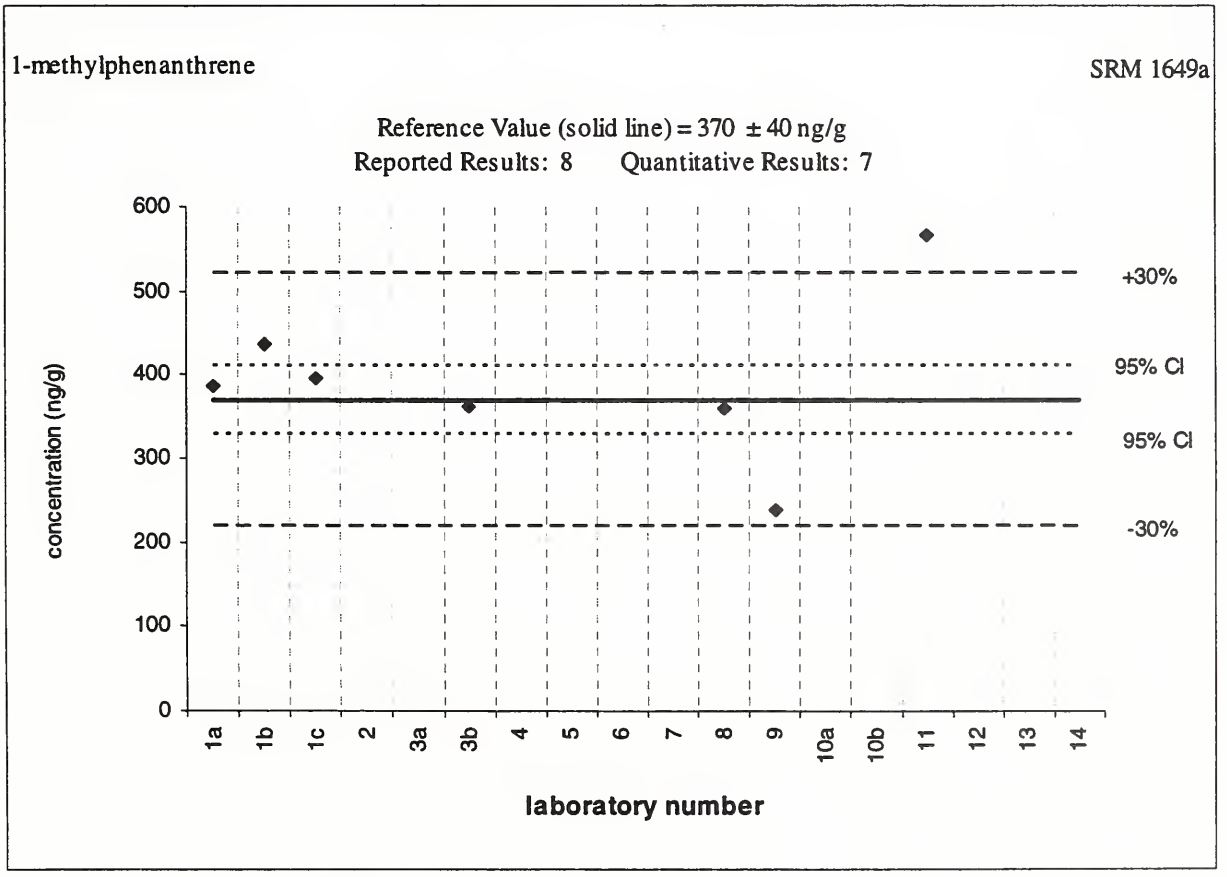
SRM 1649a

Reference Value (solid line) = 370 ± 40 ng/g

Reported Results: 8 Quantitative Results: 7




1-methylphenanthrene
Baltimore 2 PM
Assigned value (solid line) = 156 ng/g s = 74 ng/g 95% CL = 92 ng/g
Reported Results: 7 Quantitative Results: 6
concentration (ng/g)
500
450
400
350
300
250
200
150
100
50
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

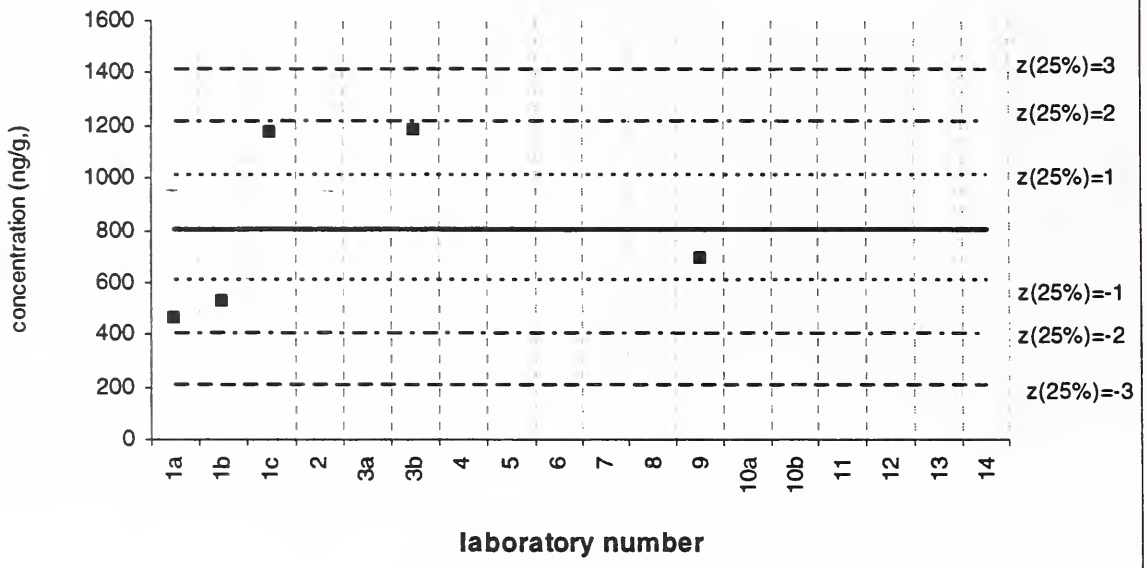

1-methylphenanthrene
SRM 1649a
Reference Value (solid line) = 370 ± 40 ng/g
Reported Results: 8 Quantitative Results: 7
concentration (ng/g)
600
500
400
300
200
100
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

1-methylphenanthrene

Filter samples

Assigned value (solid line) = 808 ng/g s = 349 ng/g 95% CL = 433 ng/g

Reported Results: 8 Quantitative Results: 5

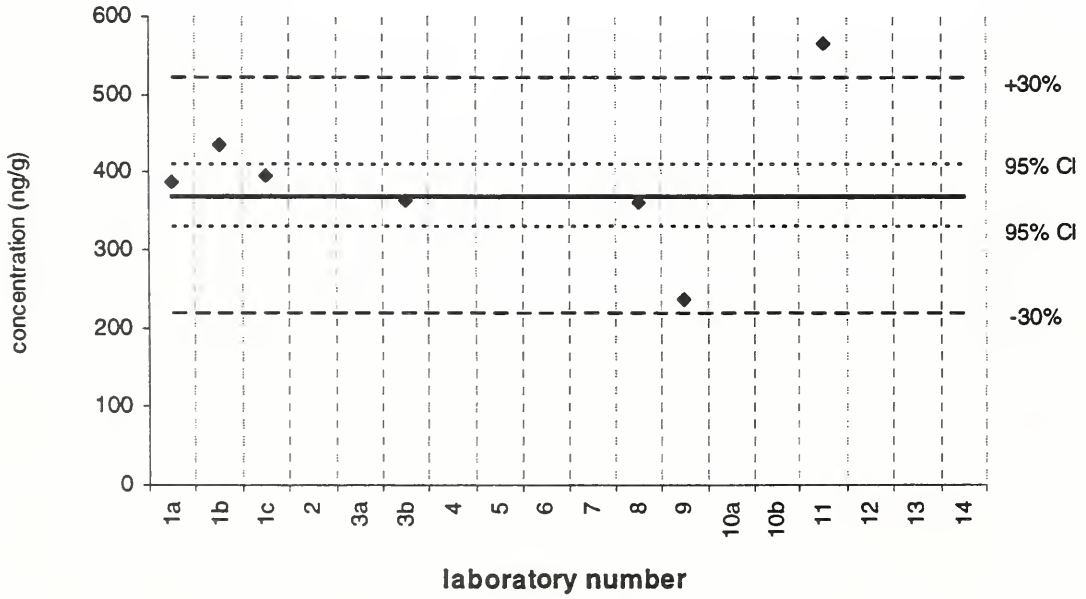


1-methylphenanthrene

SRM 1649a

Reference Value (solid line) = 370 ± 40 ng/g

Reported Results: 8 Quantitative Results: 7

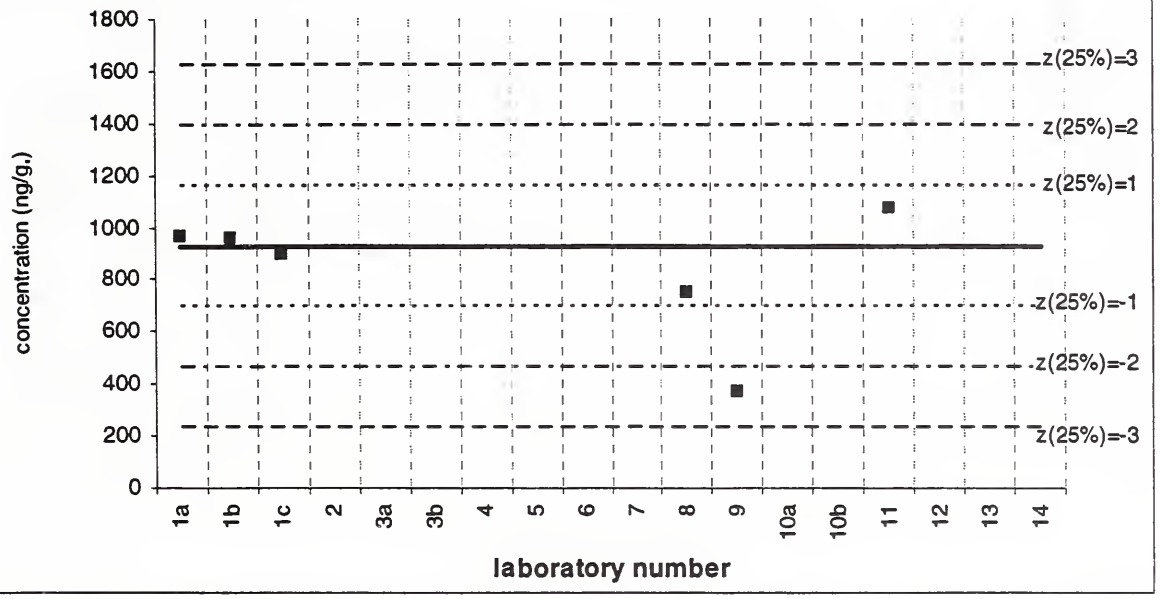


2-methylphenanthrene

SRM 1648

Assigned value (solid line) = 928 ng/g s = 119 ng/g 95% CL = 147 ng/g

Reported Results: 7 Quantitative Results: 6

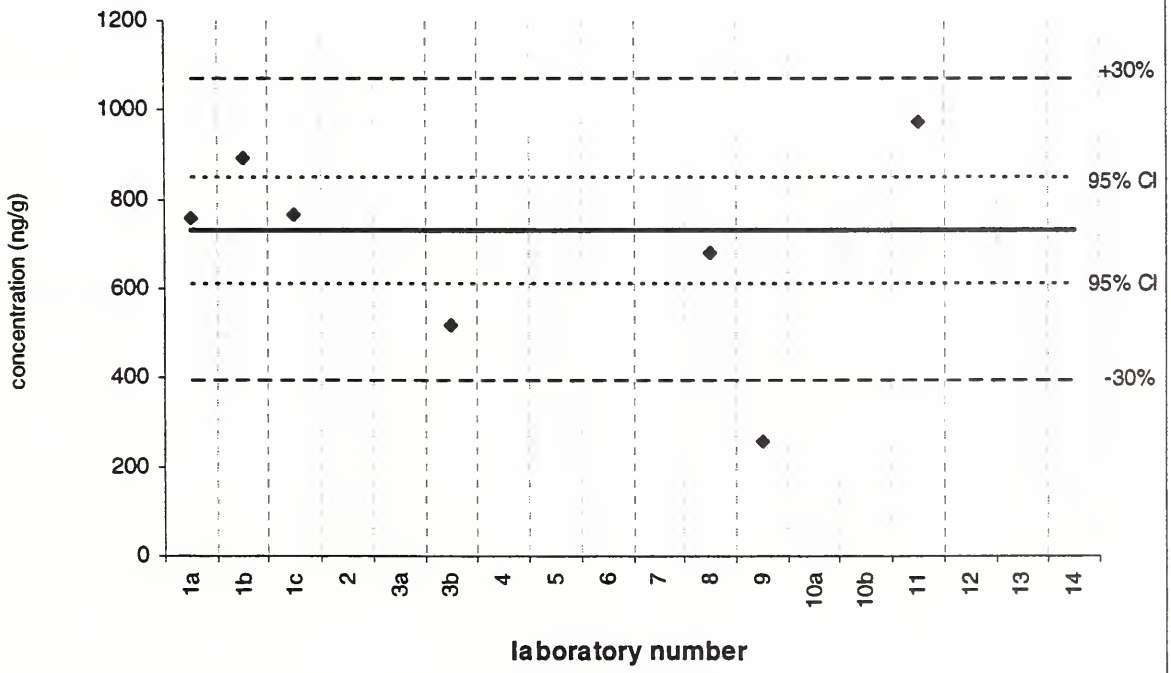


2-methylphenanthrene

SRM 1649a

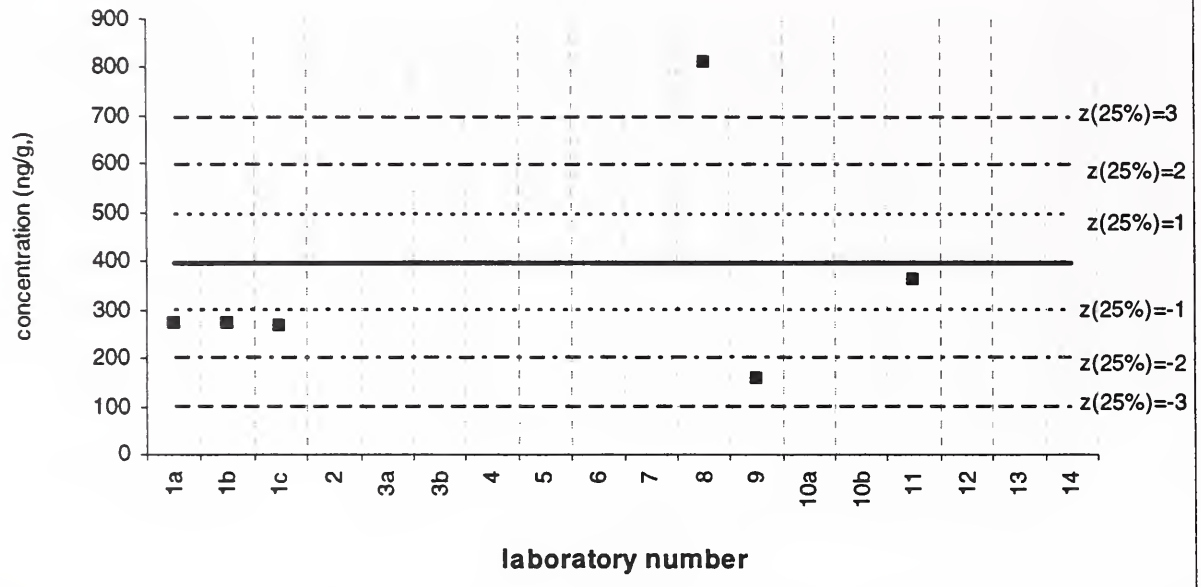
Reference Value (solid line) = 730 ± 120 ng/g

Reported Results: 8 Quantitative Results: 7



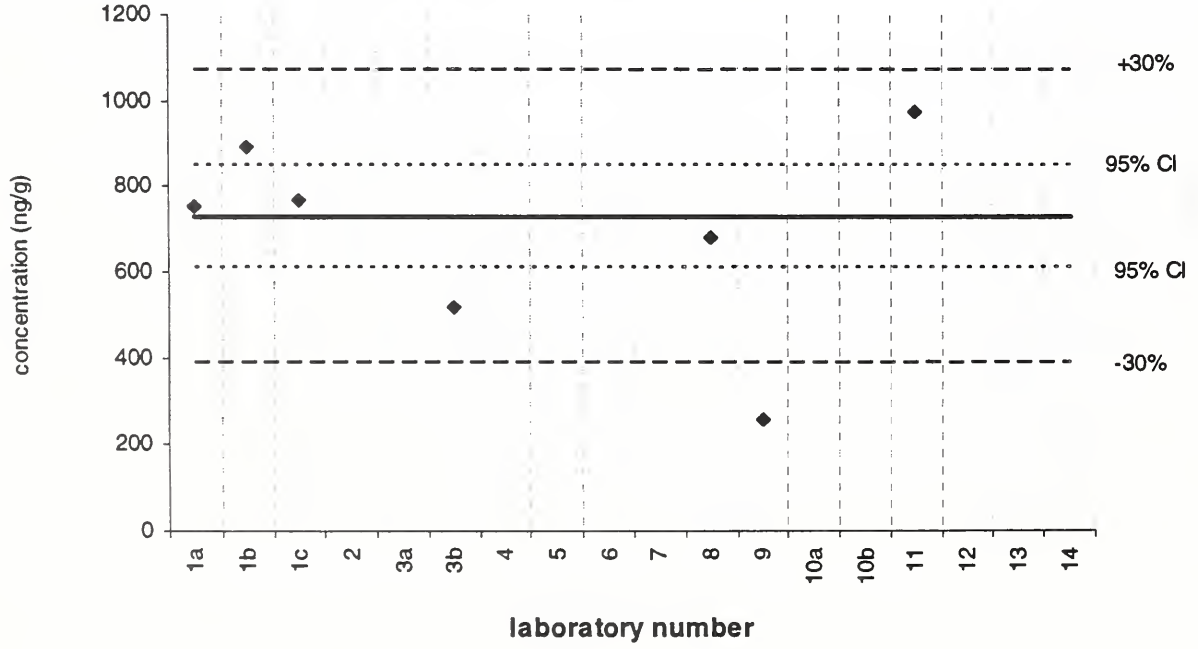
2-methylphenanthrene Baltimore 2 PM

Assigned value (solid line) = 397 ng/g s = 234 ng/g 95% CL = 290 ng/g
Reported Results: 7 Quantitative Results: 6



2-methylphenanthrene SRM 1649a

Reference Value (solid line) = 730 ± 120 ng/g
Reported Results: 8 Quantitative Results: 7

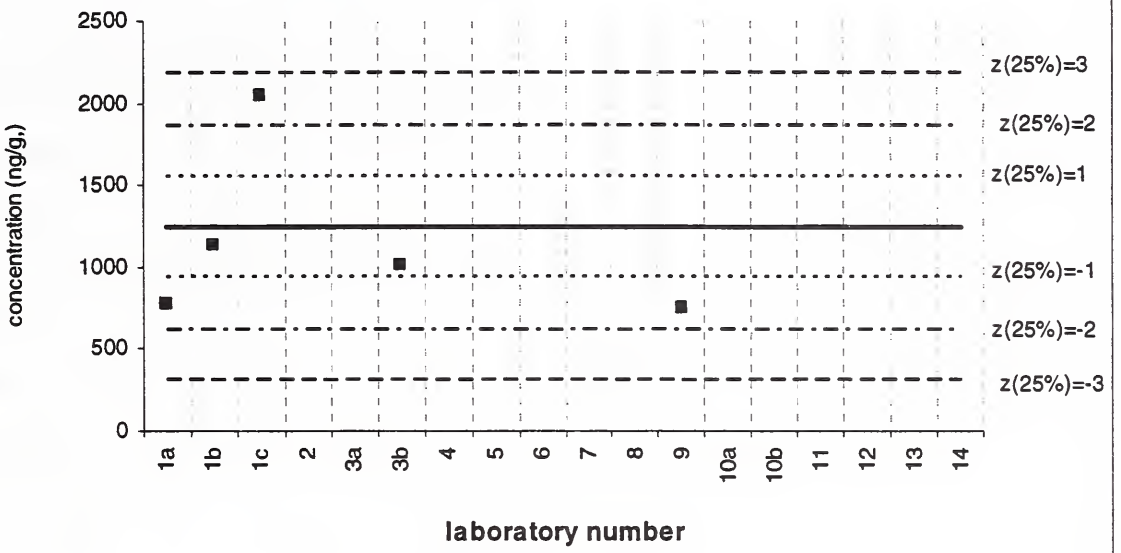


2-methylphenanthrene

Filter samples

Assigned value (solid line) = 1243 ng/g s = 556 ng/g 95% CL = 885 ng/g

Reported Results: 8 Quantitative Results: 5

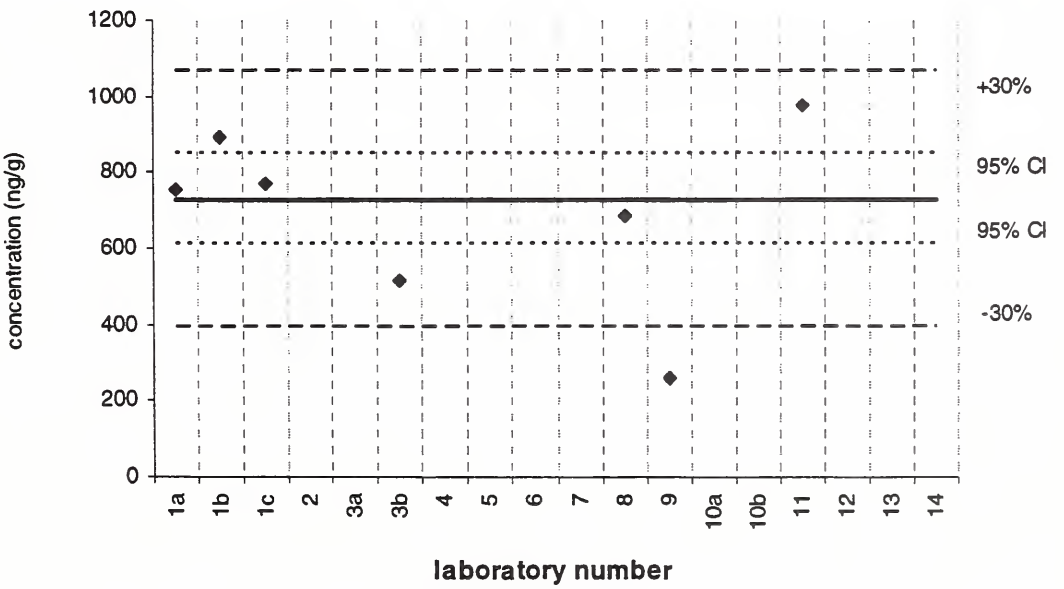


2-methylphenanthrene

SRM 1649a

Reference Value (solid line) = 730 ± 120 ng/g

Reported Results: 8 Quantitative Results: 7

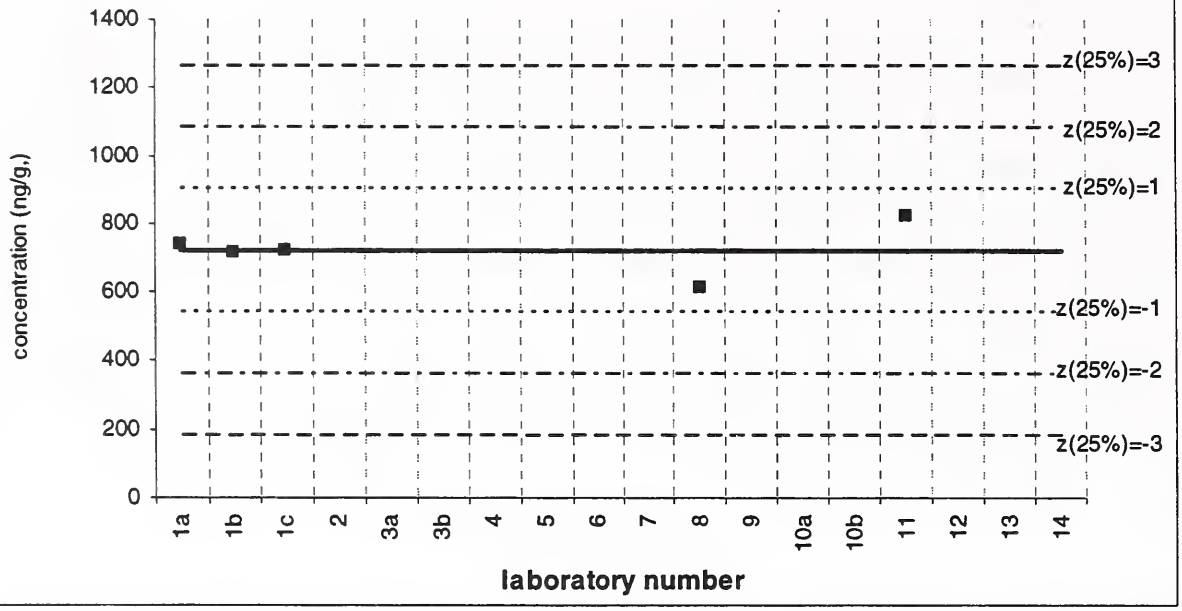


3-methylphenanthrene

SRM 1648

Assigned value (solid line) = 722 ng/g s = 76 ng/g 95% CL = 94 ng/g

Reported Results: 7 Quantitative Results: 5

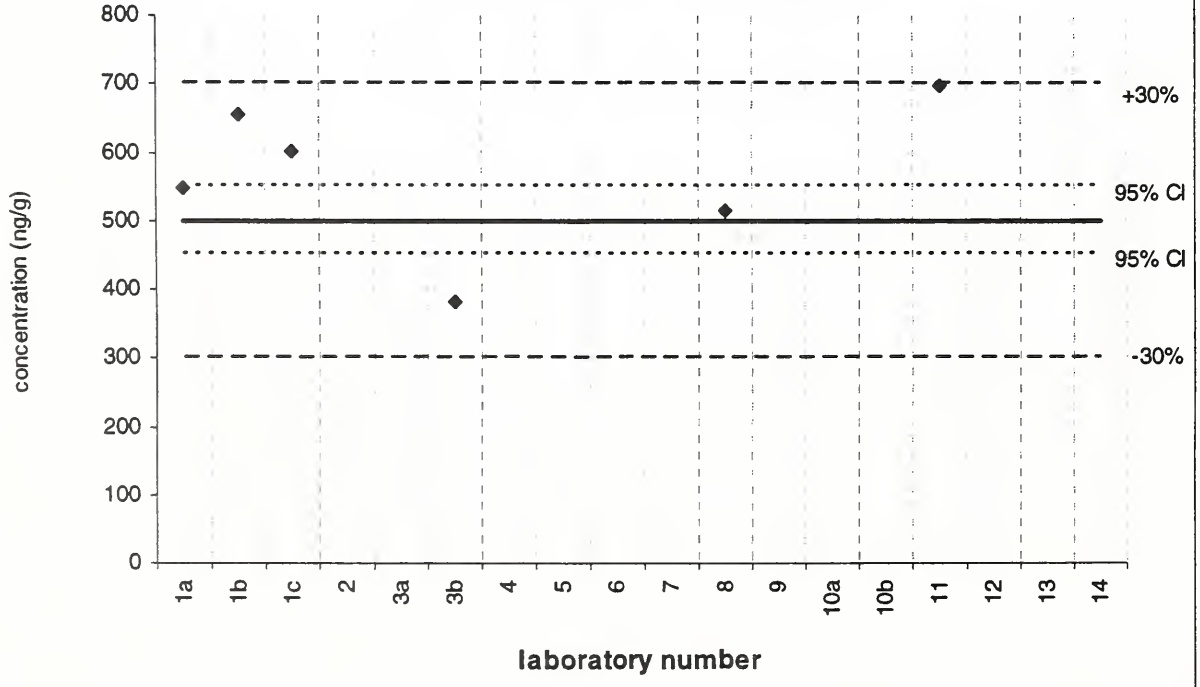


3-methylphenanthrene

SRM 1649a

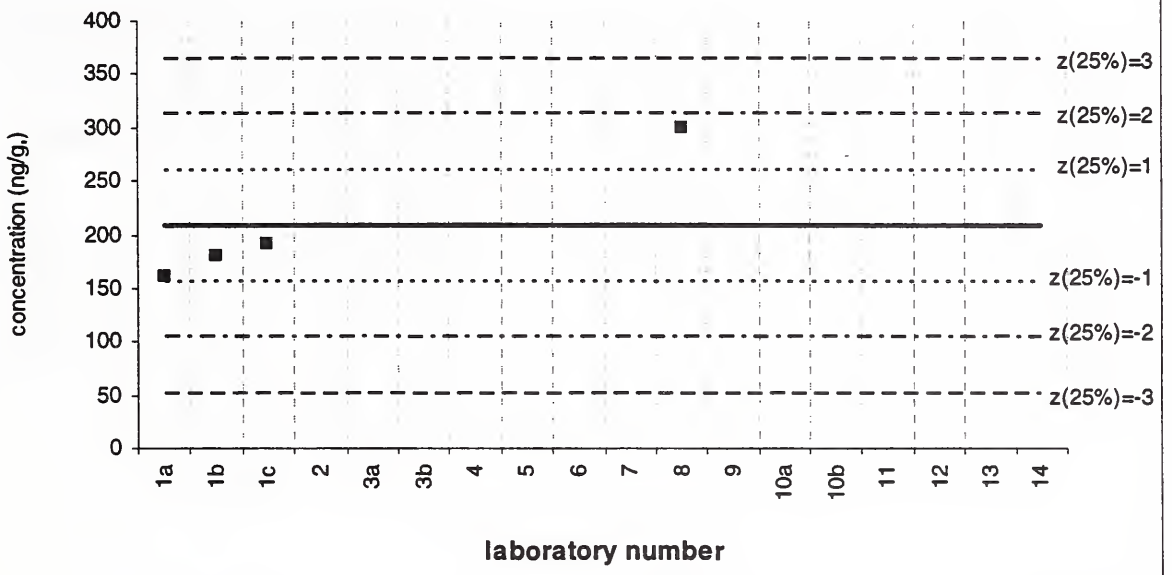
Reference Value (solid line) = 500 ± 50 ng/g

Reported Results: 8 Quantitative Results: 6



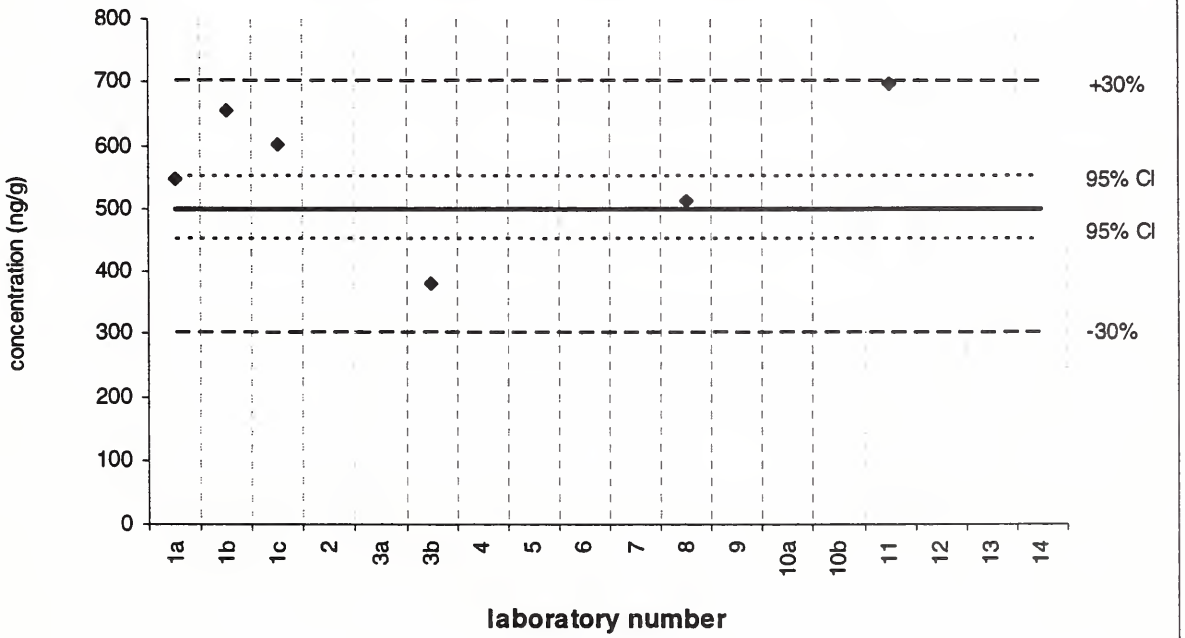
3-methylphenanthrene Baltimore 2 PM

Assigned value (solid line) = 208 ng/g s = 62 ng/g 95% CL = 99 ng/g
Reported Results: 7 Quantitative Results: 4



3-methylphenanthrene SRM 1649a

Reference Value (solid line) = 500 ± 50 ng/g
Reported Results: 8 Quantitative Results: 6

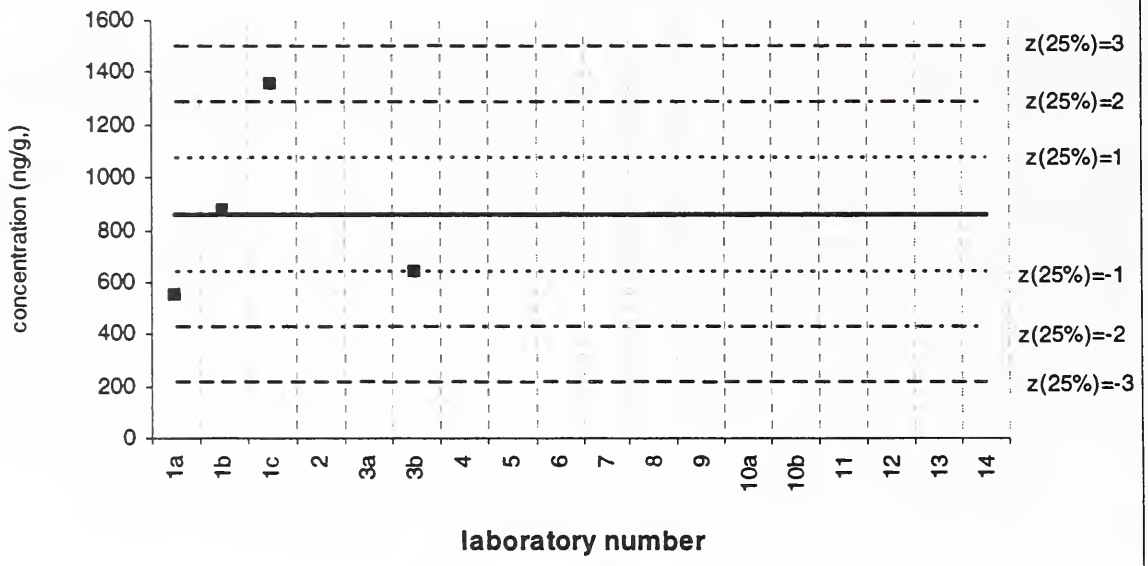


3-methylphenanthrene

Filter samples

Assigned value (solid line) = 856 ng/g s = 360 ng/g 95% CL = 573 ng/g

Reported Results: 8 Quantitative Results: 4

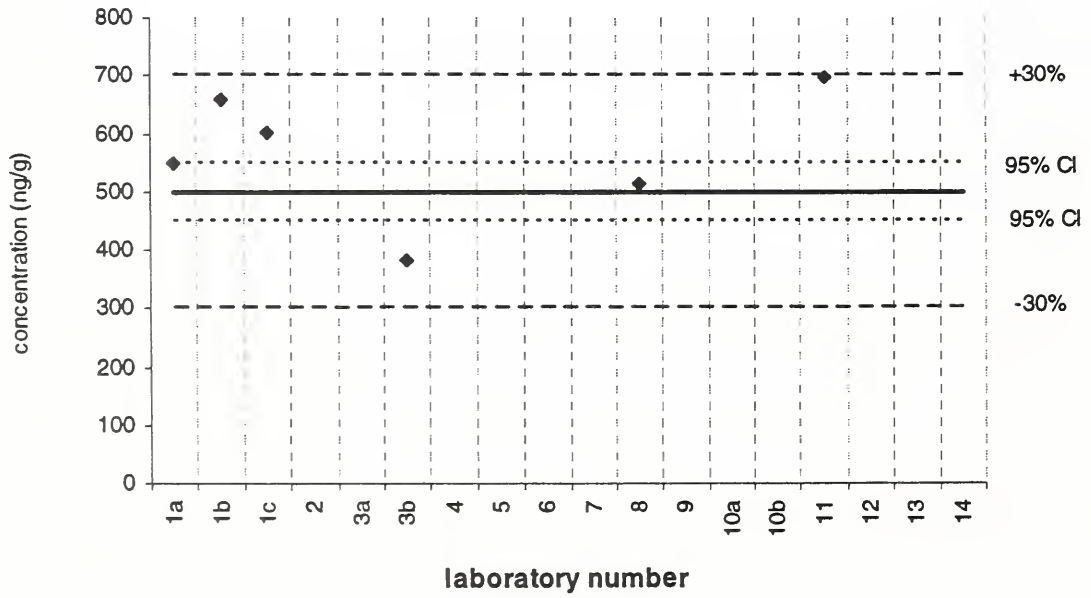


3-methylphenanthrene

SRM 1649a

Reference Value (solid line) = 500 ± 50 ng/g

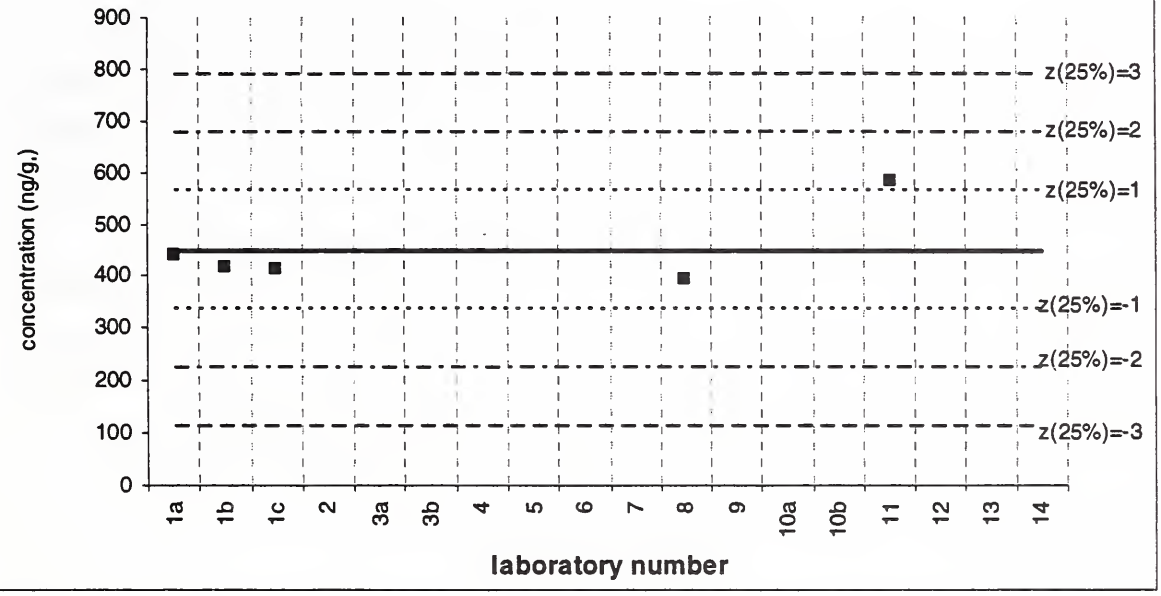
Reported Results: 8 Quantitative Results: 6



9-methylphenanthrene SRM 1648

Assigned value (solid line) = 450 ng/g s = 76 ng/g 95% CL = 94 ng/g

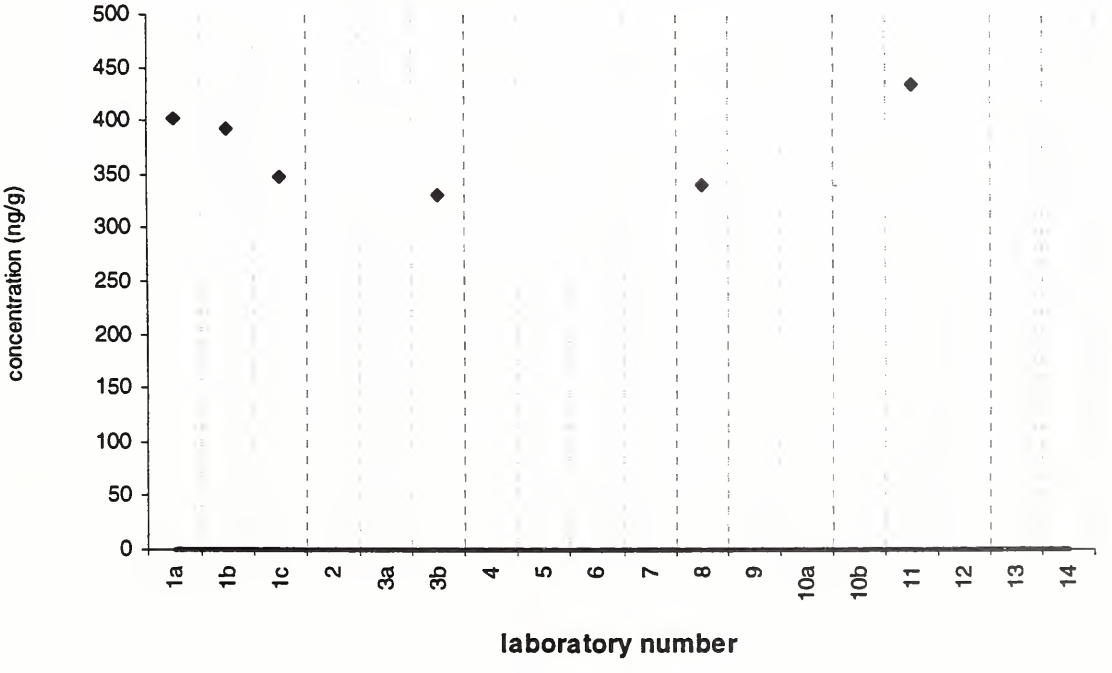
Reported Results: 7 Quantitative Results: 5



9-methylphenanthrene SRM 1649a

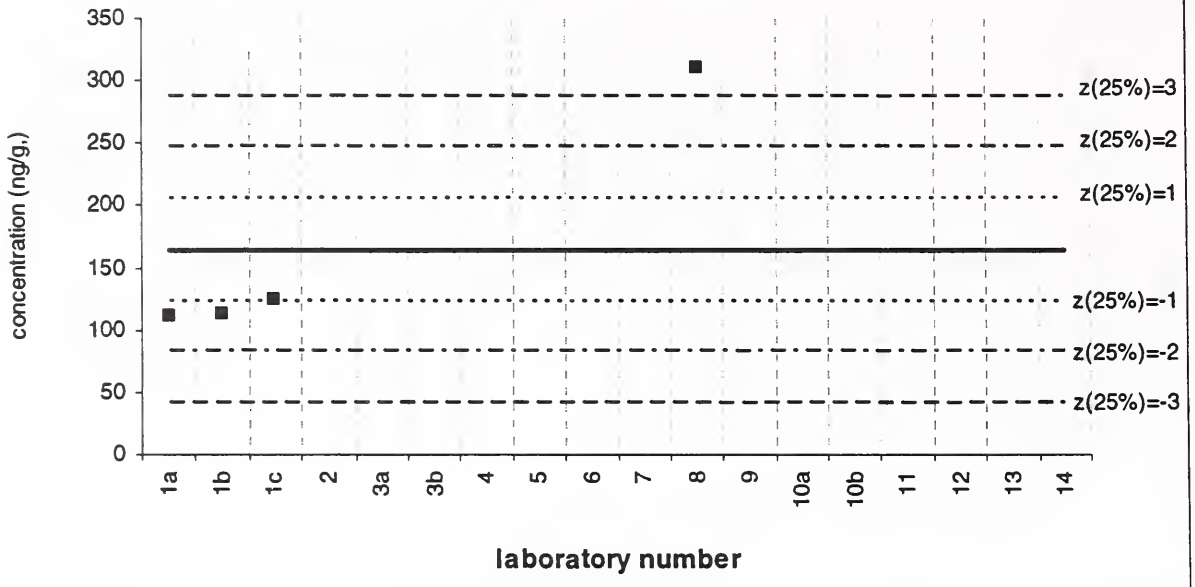
Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 6



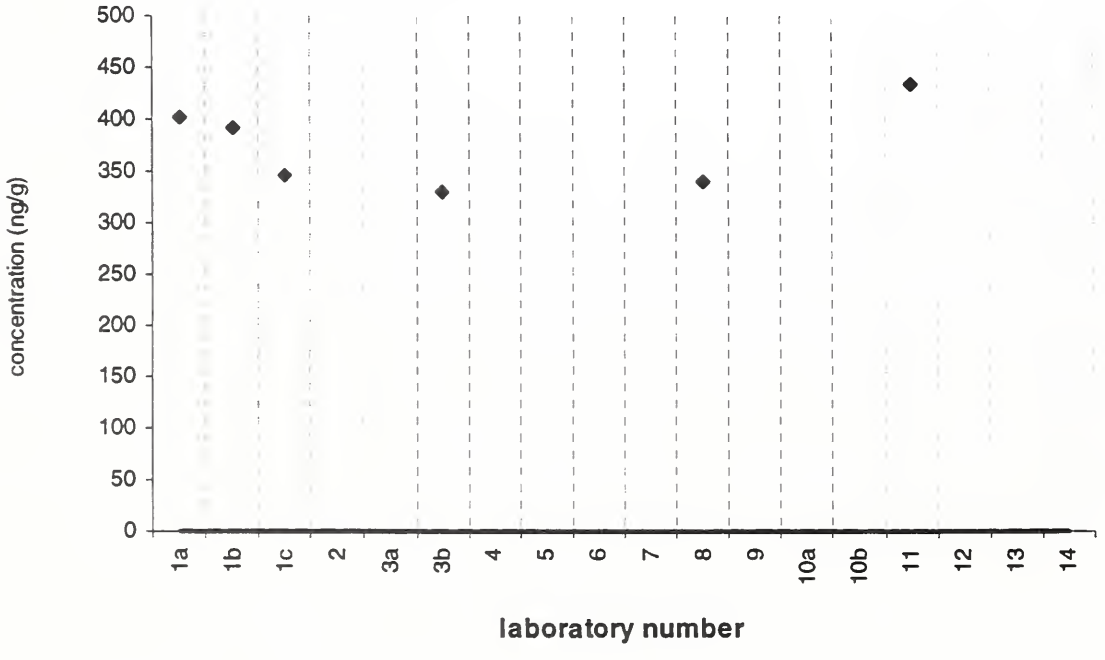
9-methylphenanthrene Baltimore 2 PM

Assigned value (solid line) = 164 ng/g s = 97 ng/g 95% CL = 155 ng/g
Reported Results: 7 Quantitative Results: 4



9-methylphenanthrene SRM 1649a

Target Value = no target ng/g
Reported Results: 8 Quantitative Results: 6

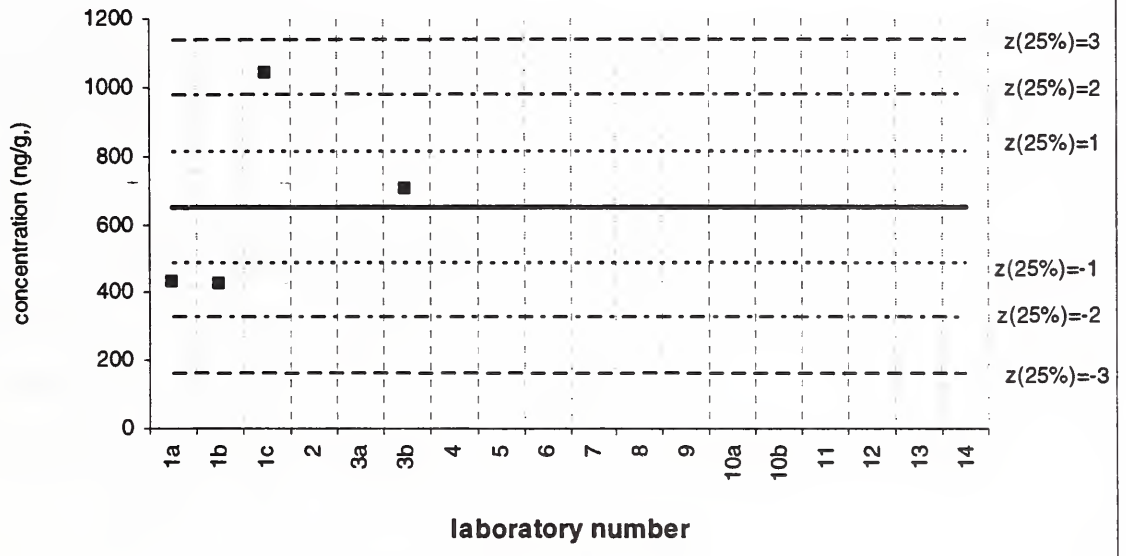


9-methylphenanthrene

Filter samples

Assigned value (solid line) = 650 ng/g s = 288 ng/g 95% CL = 459 ng/g

Reported Results: 8 Quantitative Results: 4

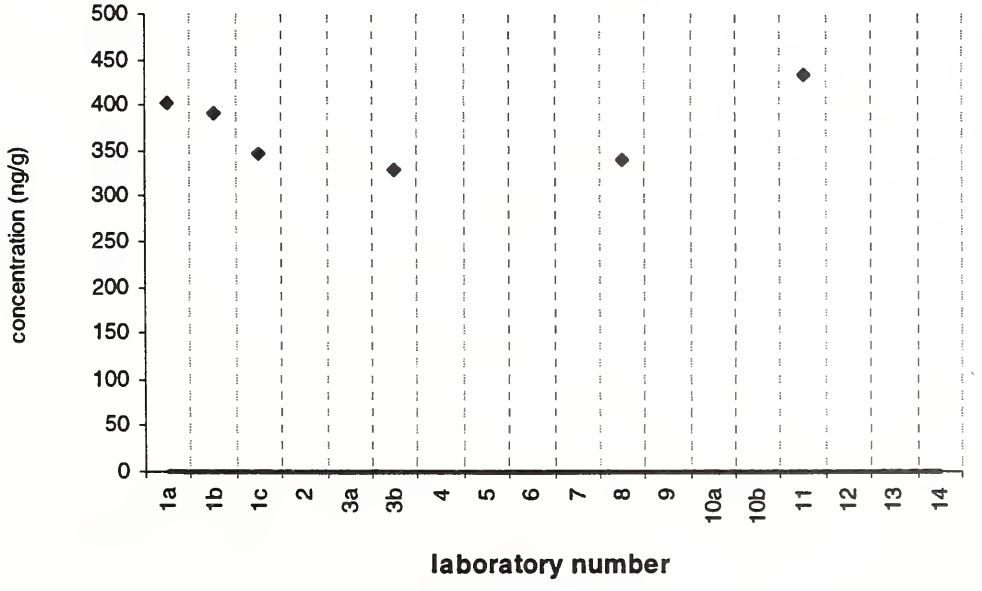


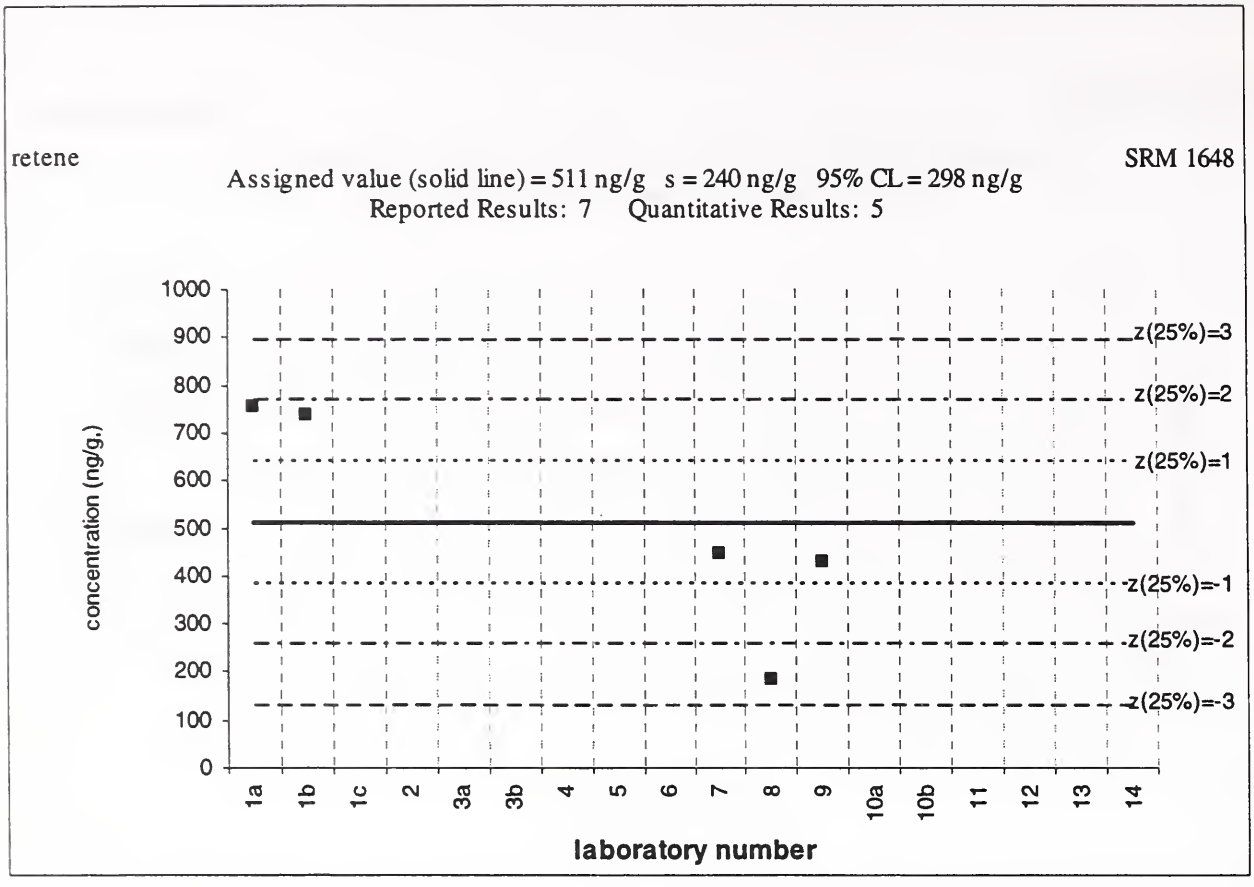
9-methylphenanthrene

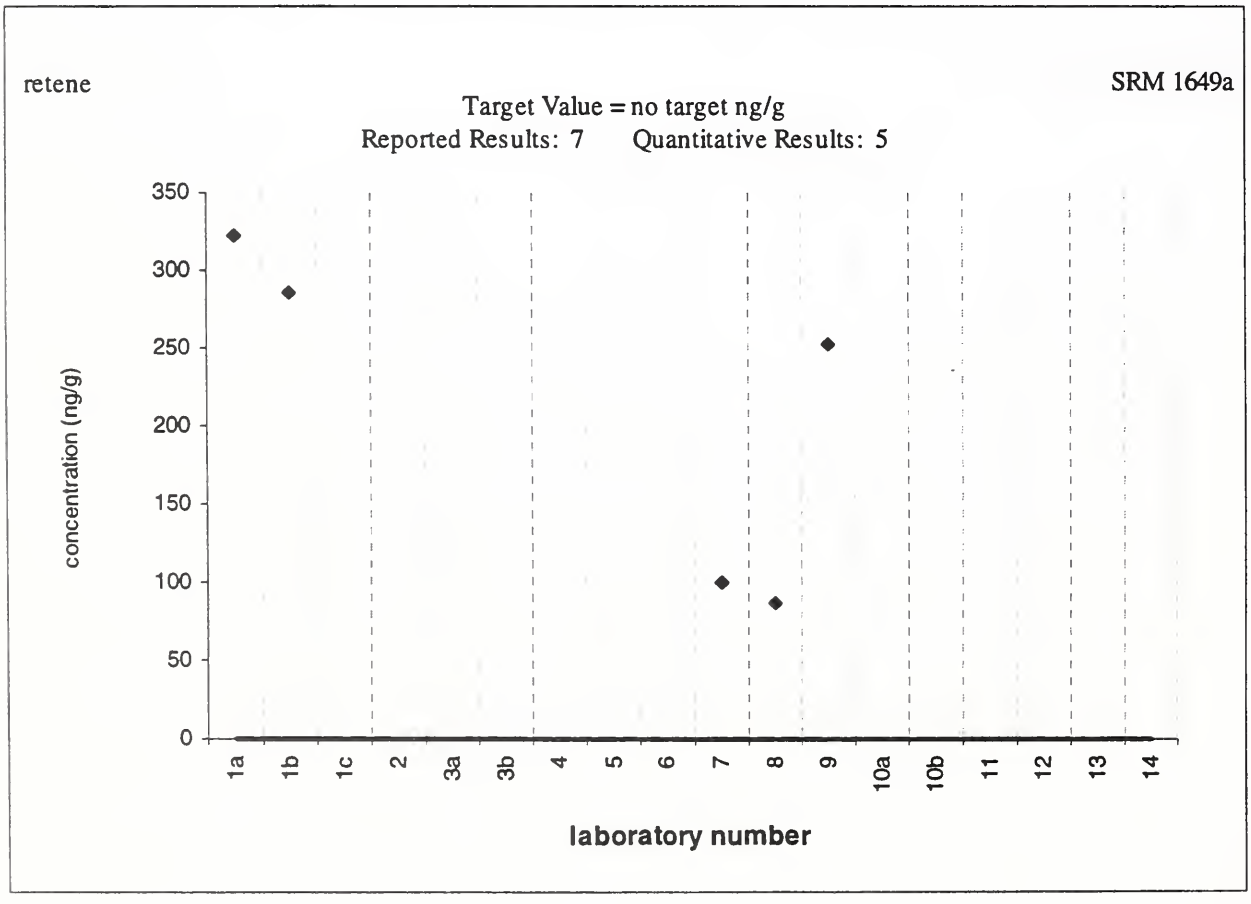
SRM 1649a

Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 6




retene
SRM 1648
Assigned value (solid line) = 511 ng/g s = 240 ng/g 95% CL = 298 ng/g
Reported Results: 7 Quantitative Results: 5
concentration (ng/g)
1000
900
800
700
600
500
400
300
200
100
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

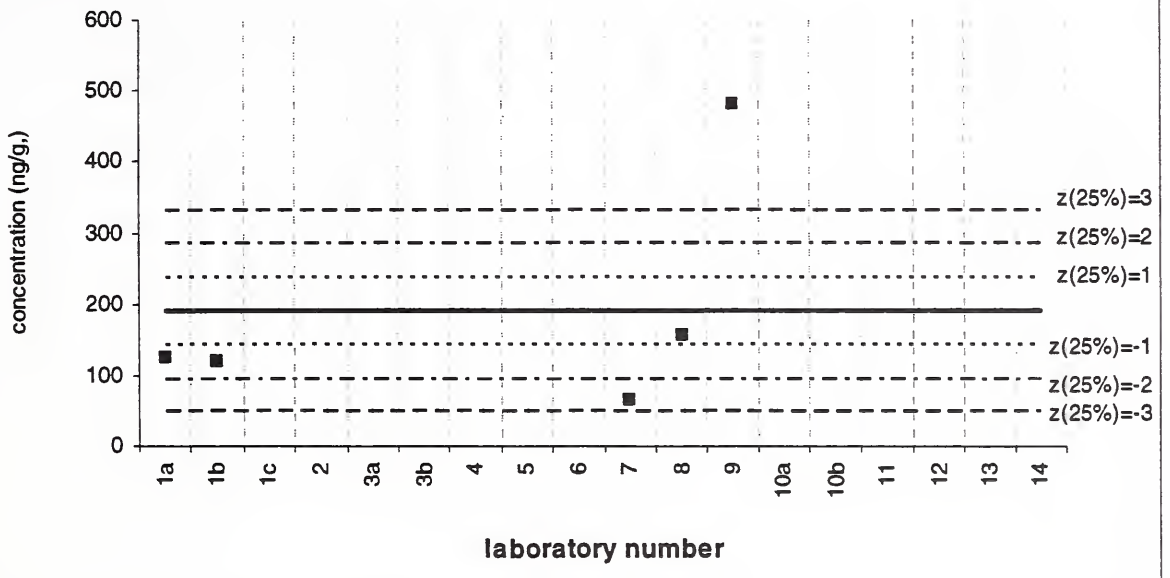

retene
SRM 1649a
Target Value = no target ng/g
Reported Results: 7 Quantitative Results: 5
concentration (ng/g)
350
300
250
200
150
100
50
0
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

retene

Baltimore 2 PM

Assigned value (solid line) = 189 ng/g s = 166 ng/g 95% CL = 206 ng/g

Reported Results: 7 Quantitative Results: 5

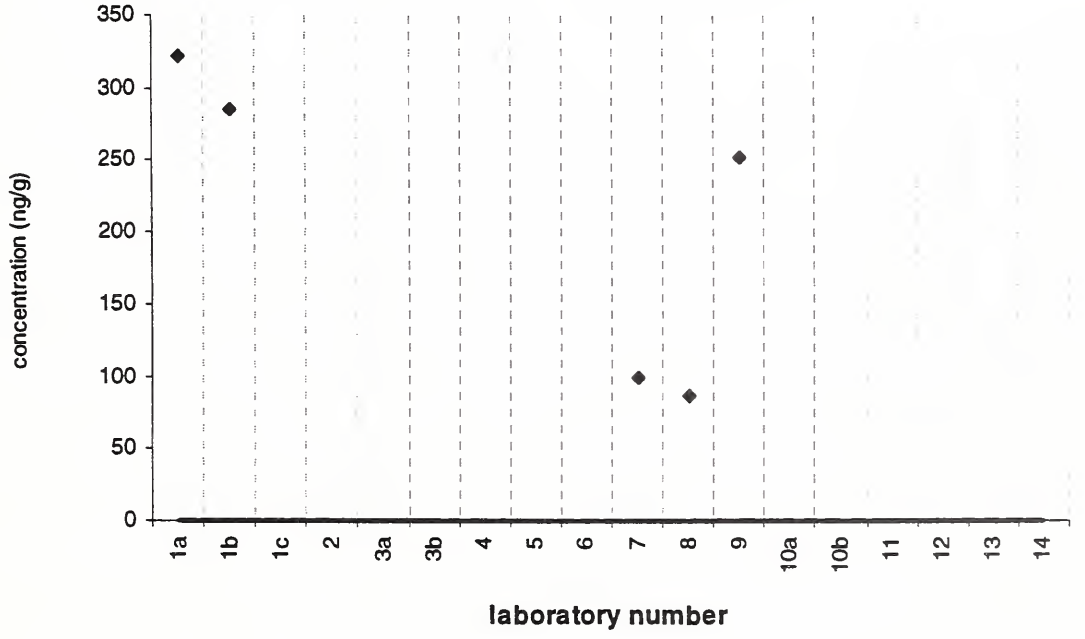


retene

SRM 1649a

Target Value = no target ng/g

Reported Results: 7 Quantitative Results: 5

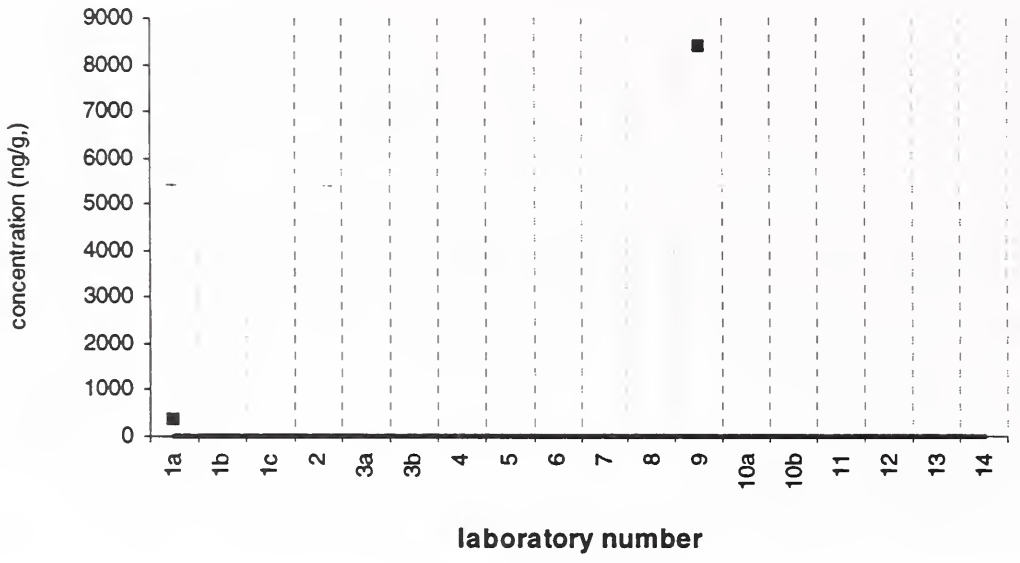


retene

Filter samples

Assigned value = no assigned value ng/g

Reported Results: 7 Quantitative Results: 2

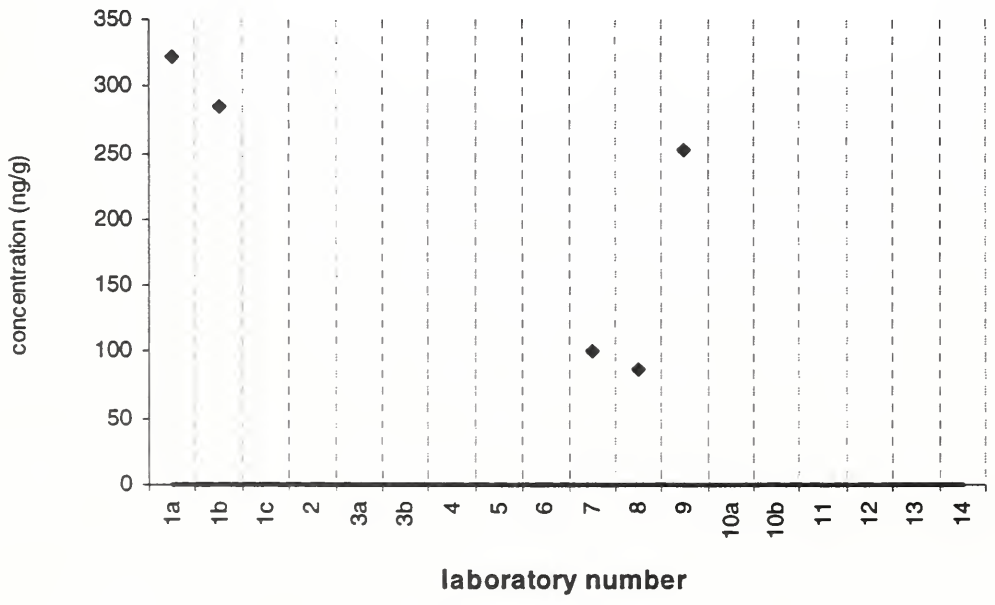


retene

SRM 1649a

Target Value = no target ng/g

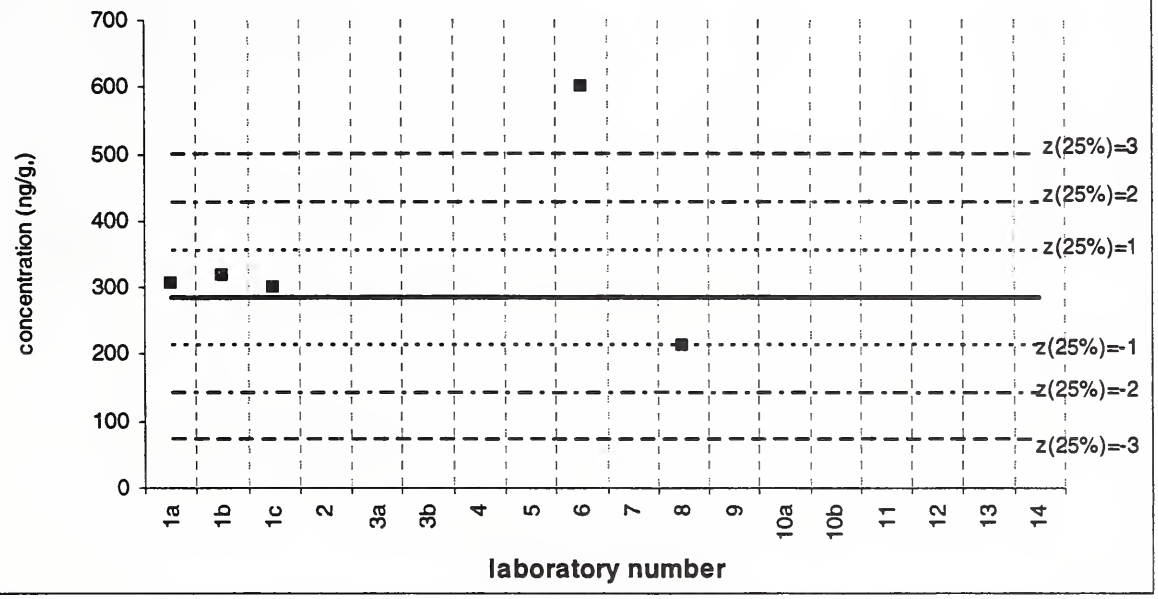
Reported Results: 7 Quantitative Results: 5



4H-cyclopenta[def]phenanthrene SRM 1648

Assigned value (solid line) = 284 ng/g s = 48 ng/g 95% CL = 76 ng/g

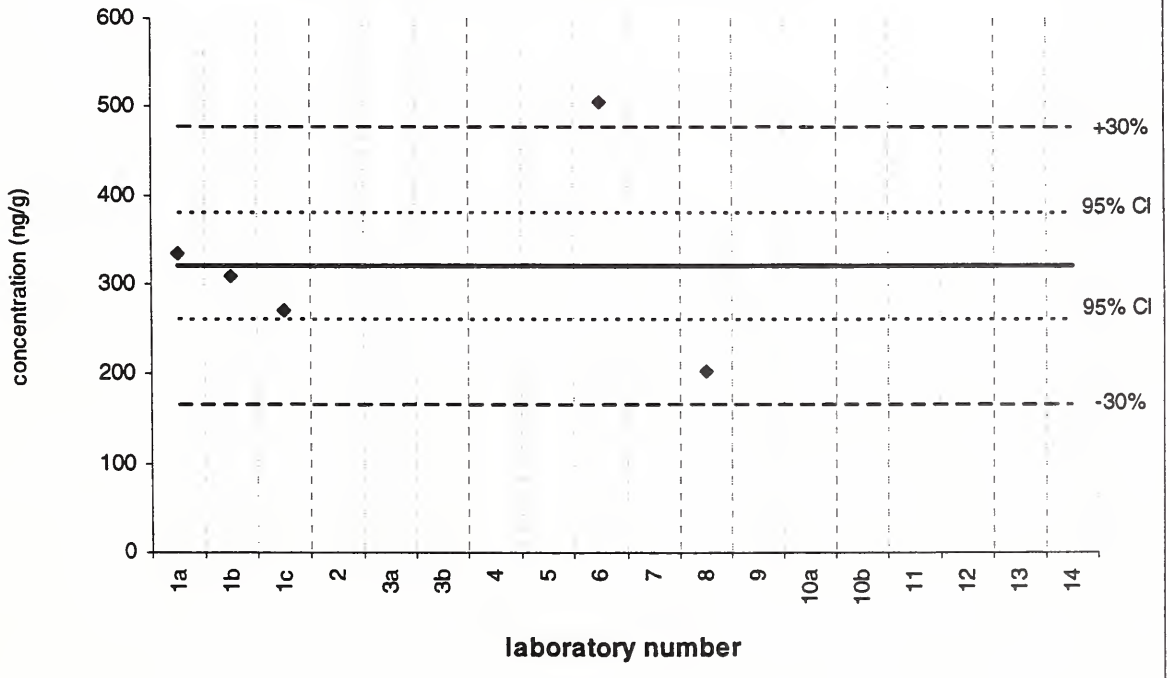
Reported Results: 6 Quantitative Results: 5



4H-cyclopenta[def]phenanthrene SRM 1649a

Reference Value (solid line) = 320 ± 60 ng/g

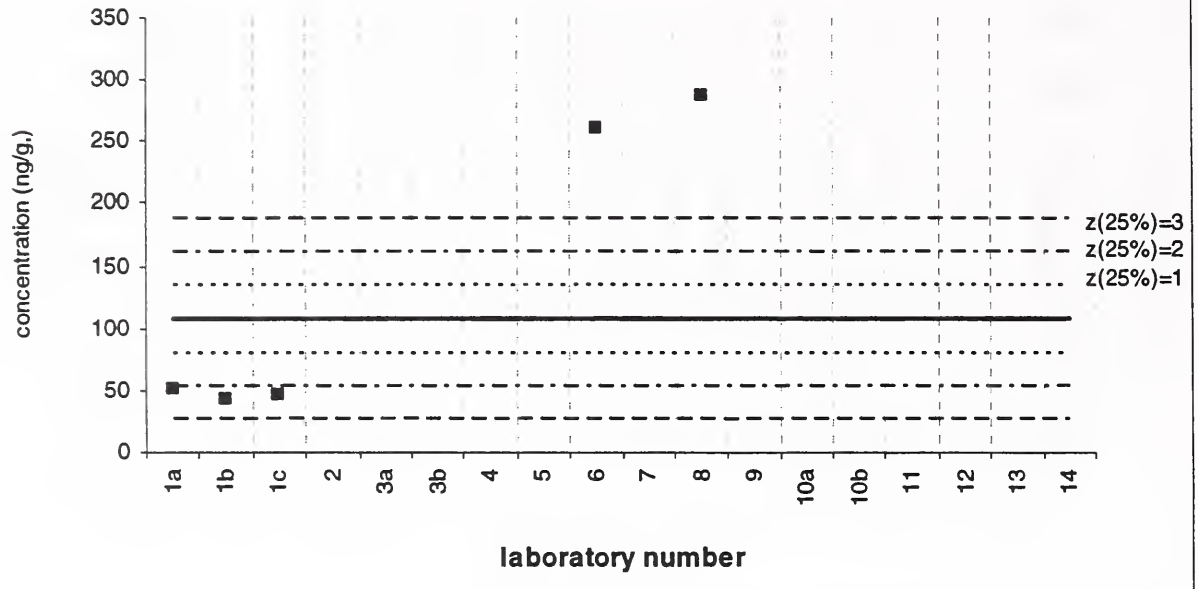
Reported Results: 6 Quantitative Results: 5



4H-cyclopenta[def]phenanthrene Baltimore 2 PM

Assigned value (solid line) = 107 ng/g s = 120 ng/g 95% CL = 191 ng/g

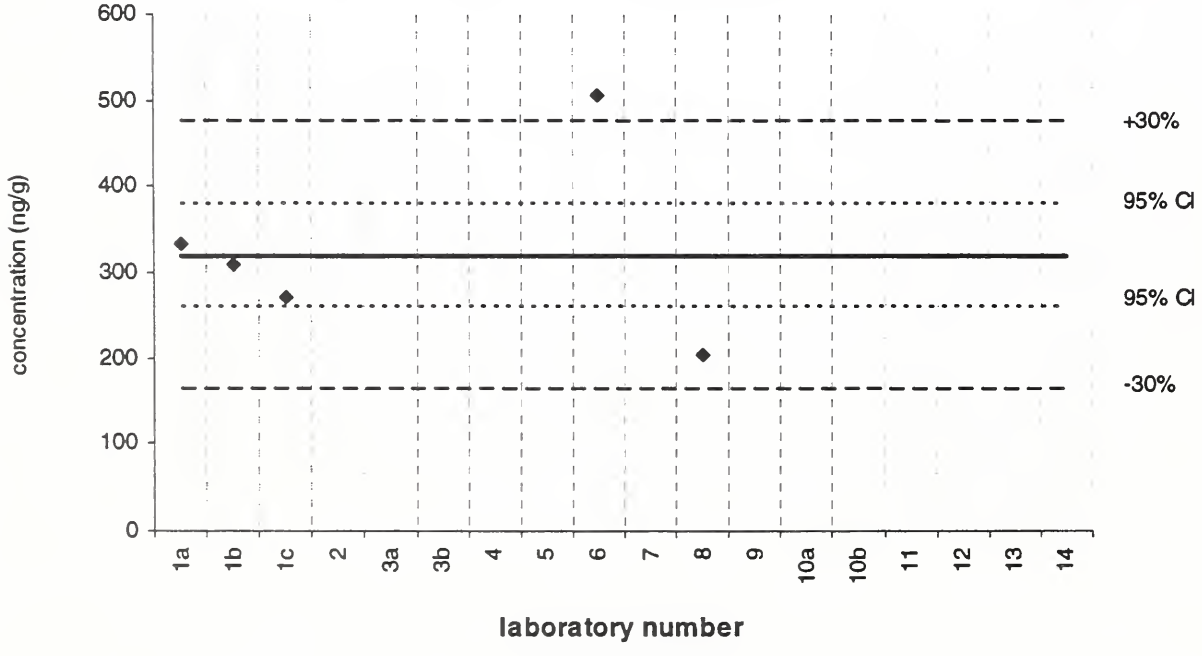
Reported Results: 6 Quantitative Results: 5



4H-cyclopenta[def]phenanthrene SRM 1649a

Reference Value (solid line) = 320 ± 60 ng/g

Reported Results: 6 Quantitative Results: 5

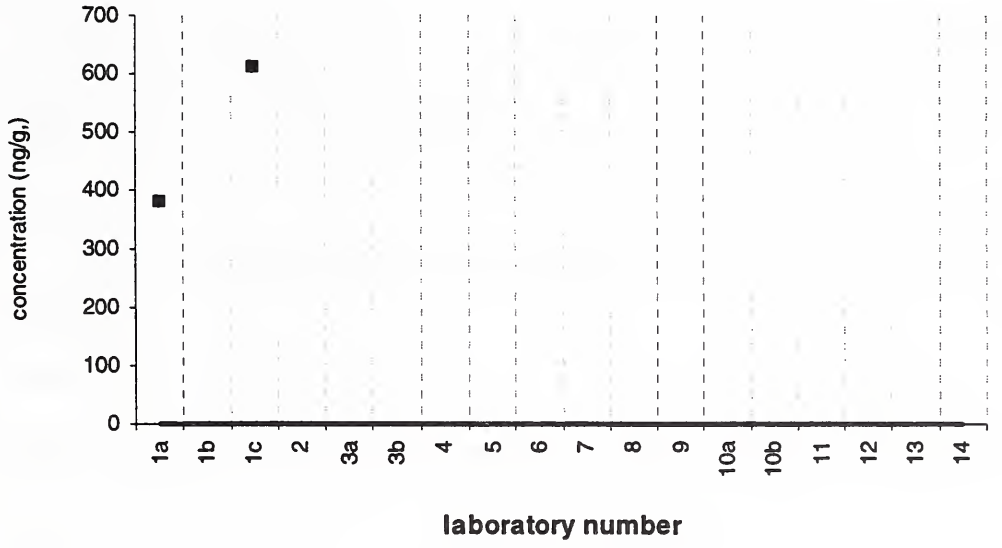


4H-cyclopenta[def]phenanthrene

Filter samples

Assigned value = no assigned value ng/g

Reported Results: 5 Quantitative Results: 2

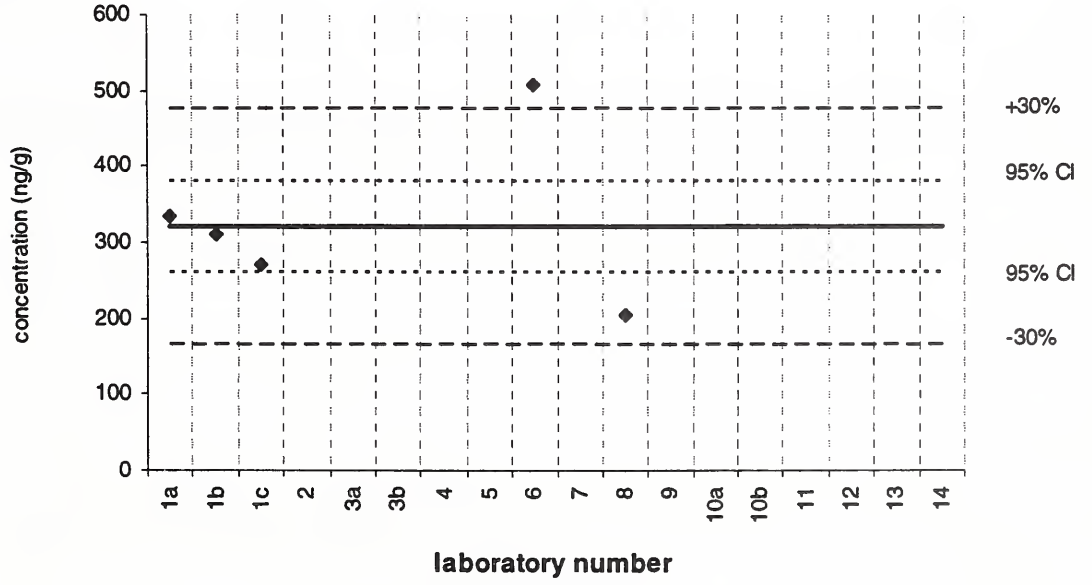


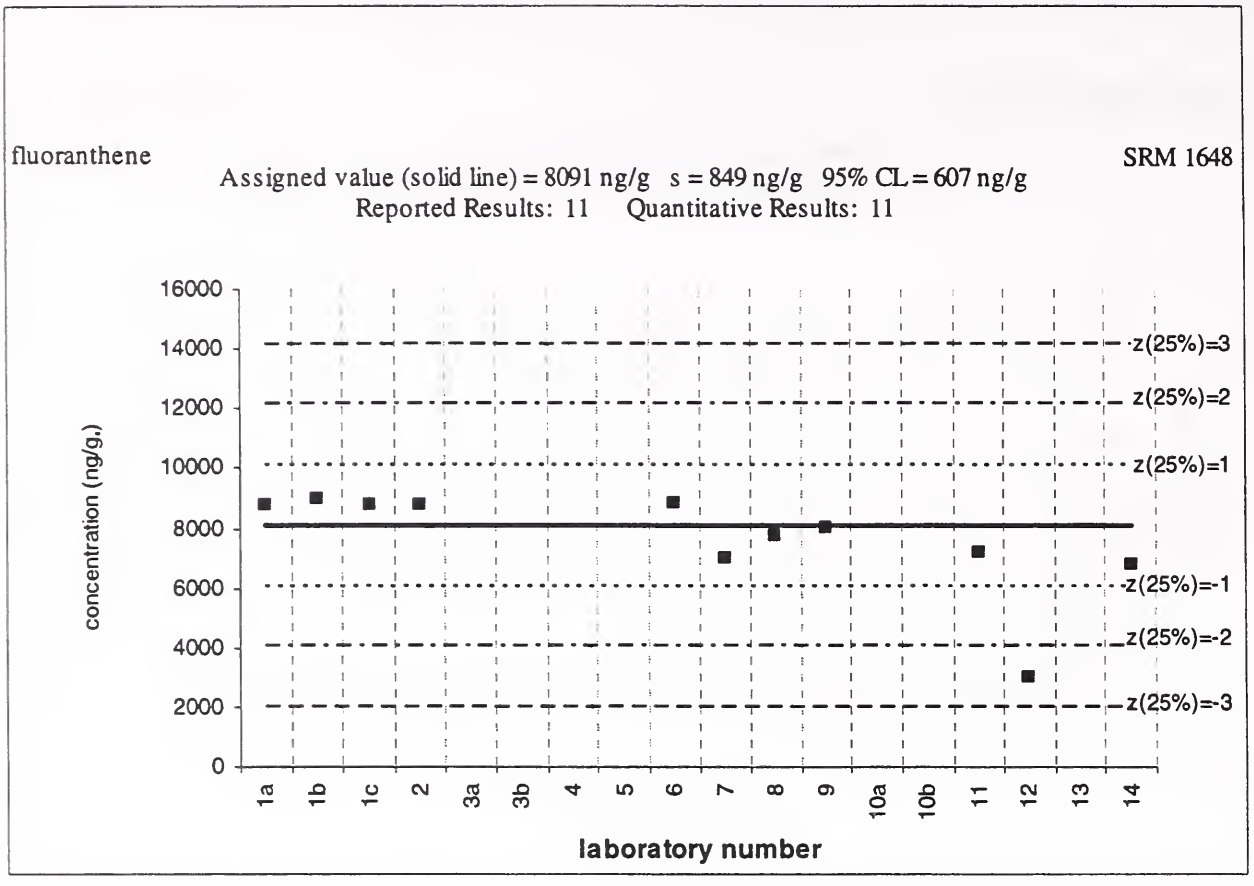
4H-cyclopenta[def]phenanthrene

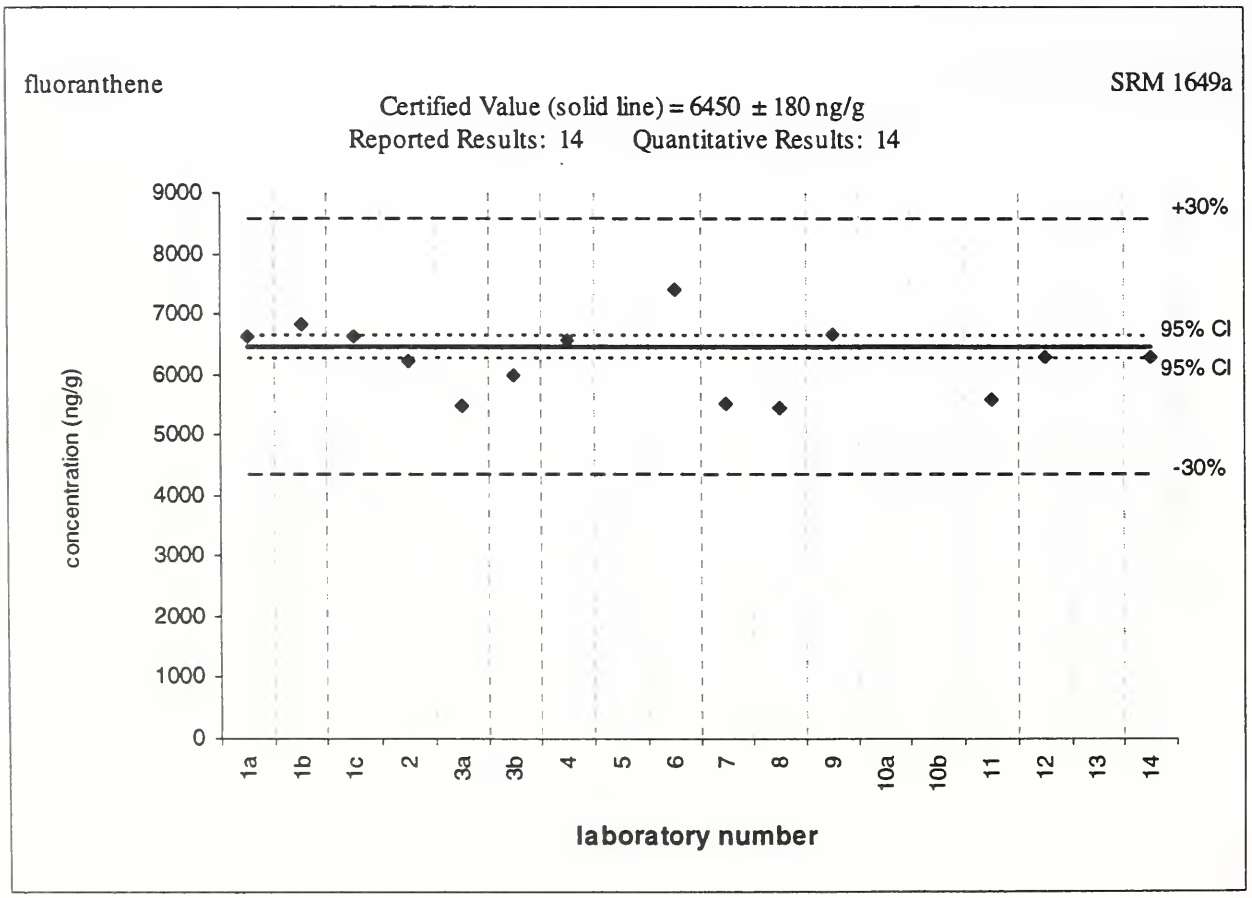
SRM 1649a

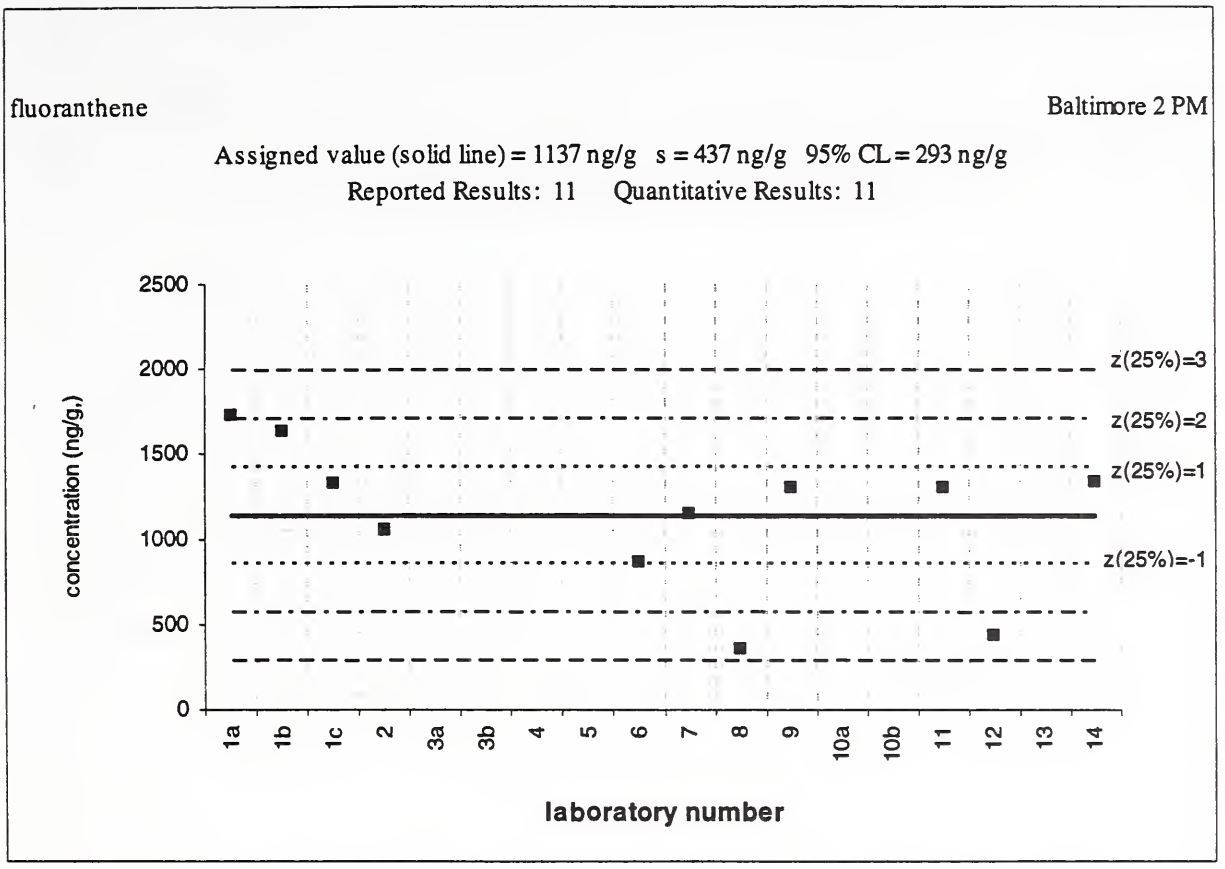
Reference Value (solid line) = 320 ± 60 ng/g

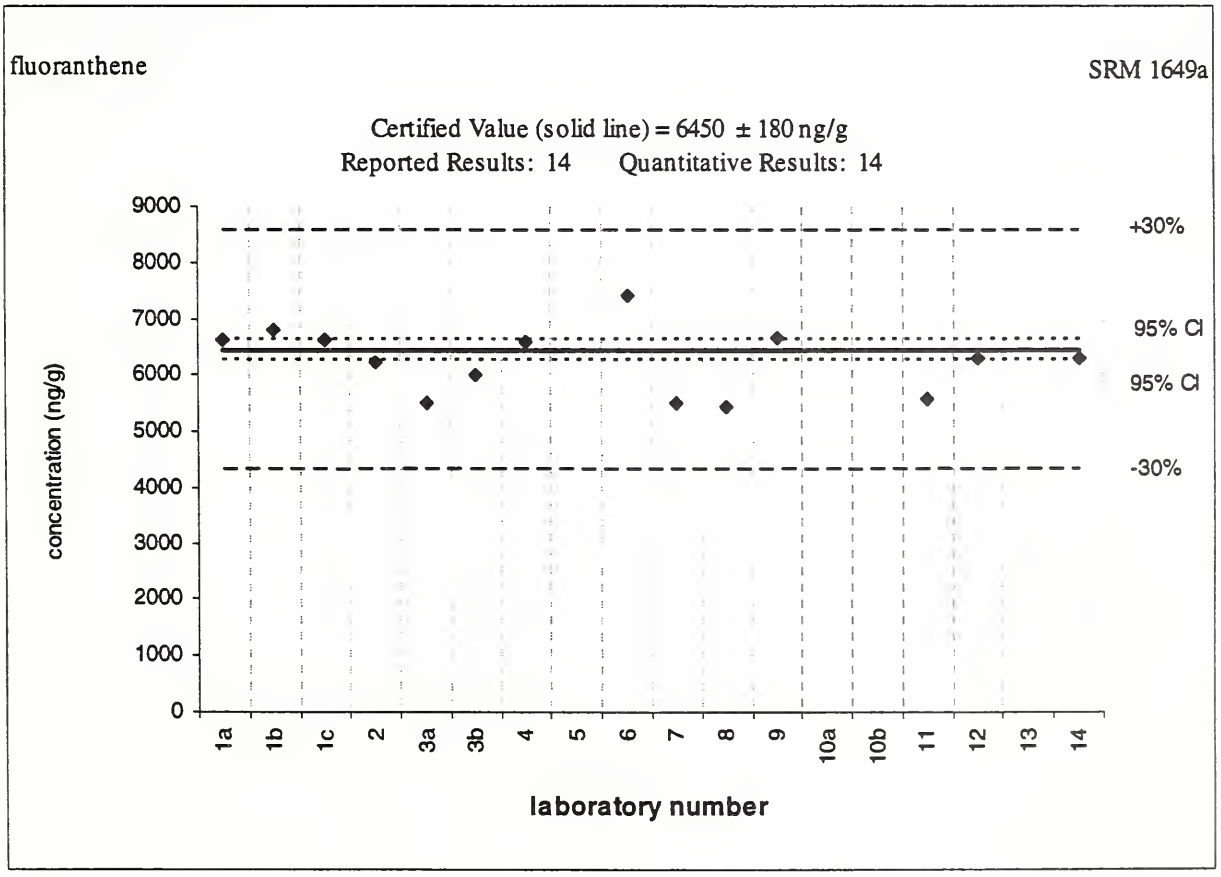
Reported Results: 7 Quantitative Results: 5




fluoranthene
SRM 1648
Assigned value (solid line) = 8091 ng/g s = 849 ng/g 95% CL = 607 ng/g
Reported Results: 11 Quantitative Results: 11
concentration (ng/g)
16000
14000
12000
10000
8000
6000
4000
2000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number


fluoranthene
SRM 1649a
Certified Value (solid line) = 6450 ± 180 ng/g
Reported Results: 14 Quantitative Results: 14
concentration (ng/g)
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% CI
95% CI
-30%
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number


fluoranthene
Baltimore 2 PM
Assigned value (solid line) = 1137 ng/g s = 437 ng/g 95% CL = 293 ng/g
Reported Results: 11 Quantitative Results: 11
concentration (ng/g,)
2500
2000
1500
1000
500
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

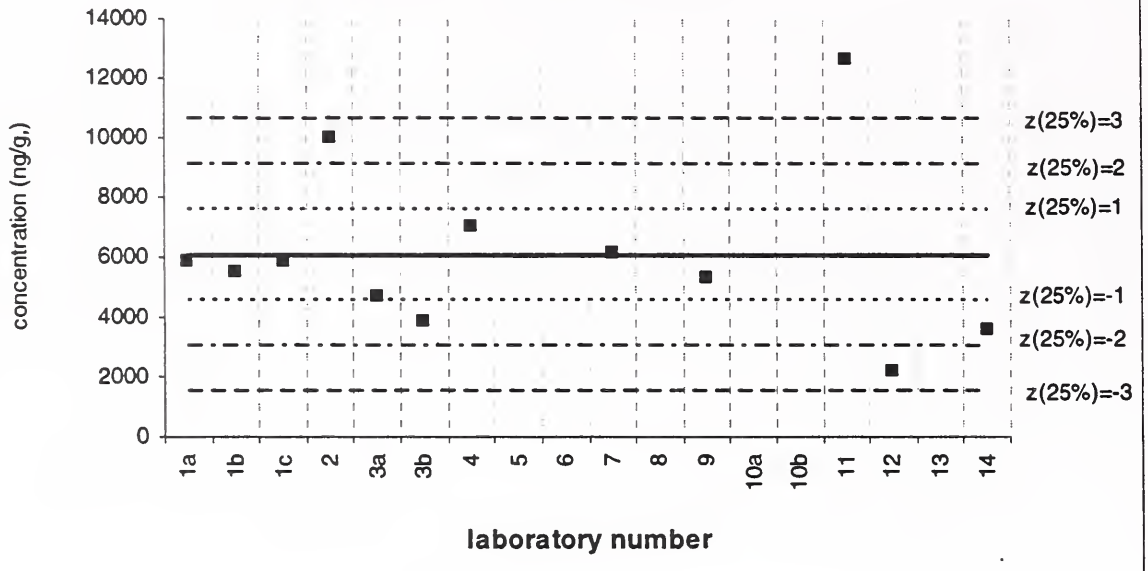

fluoranthene
SRM 1649a
Certified Value (solid line) = 6450 ± 180 ng/g
Reported Results: 14 Quantitative Results: 14
concentration (ng/g)
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

fluoranthene

Filter samples

Assigned value (solid line) = 6057 ng/g s = 2829 ng/g 95% CL = 1797 ng/g

Reported Results: 13 Quantitative Results: 12

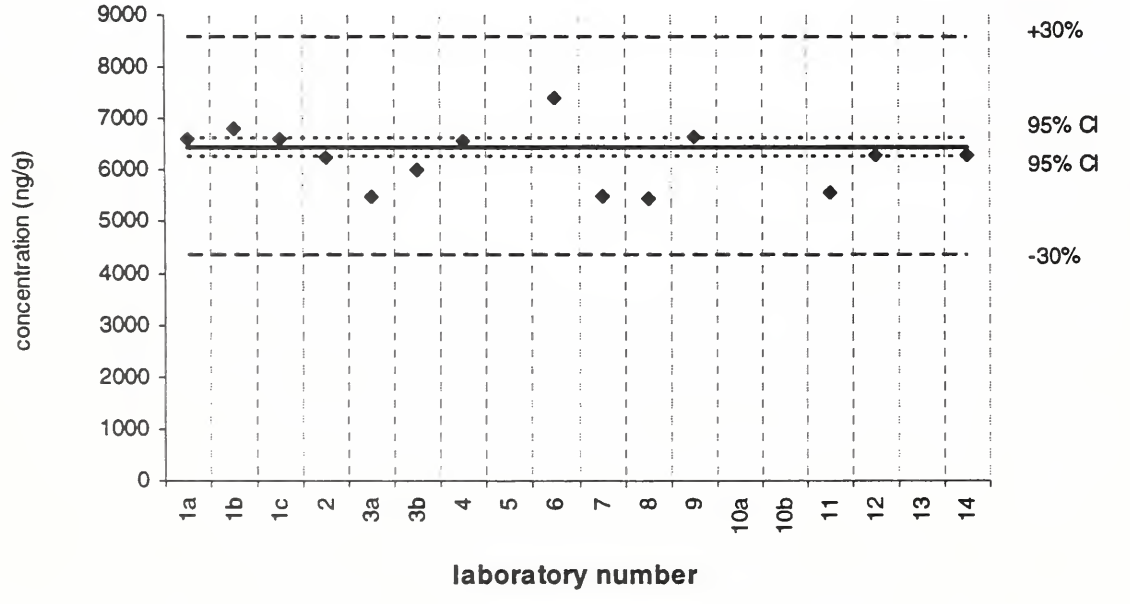


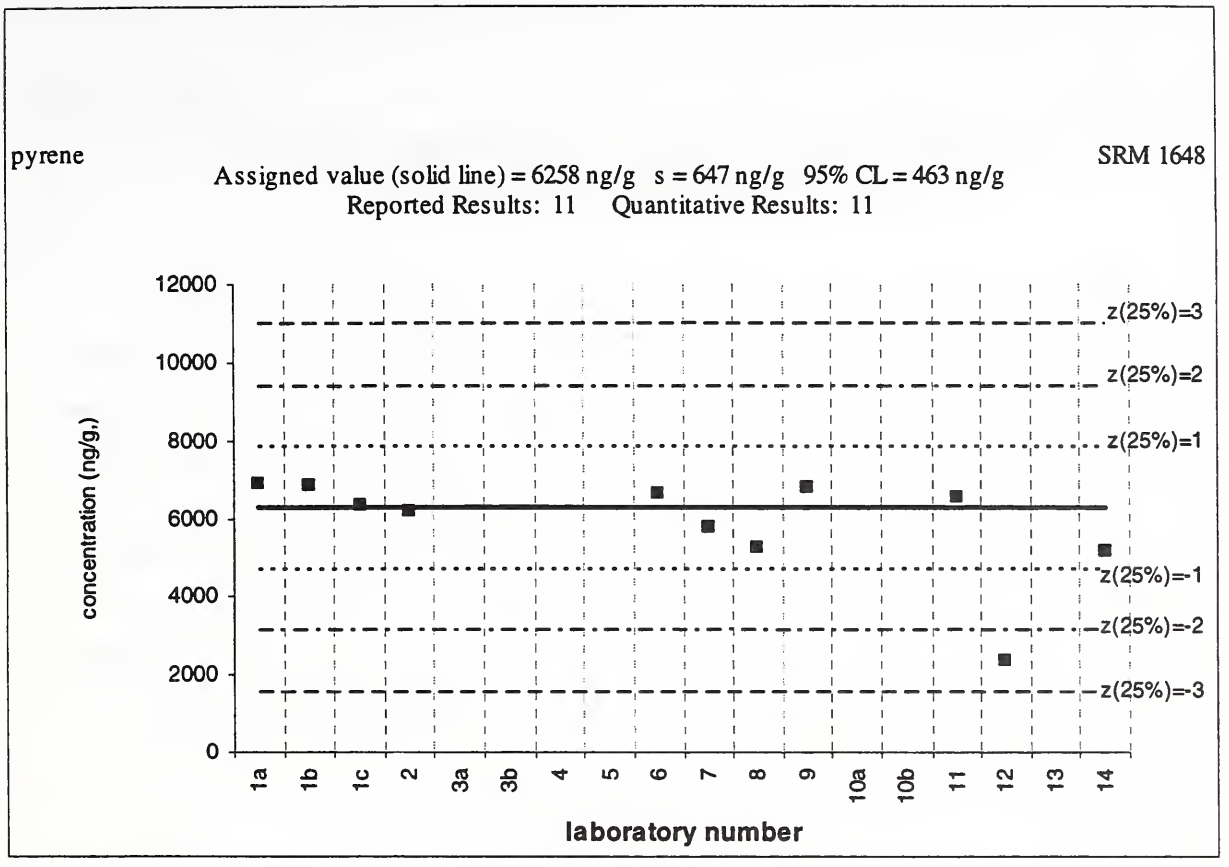
fluoranthene

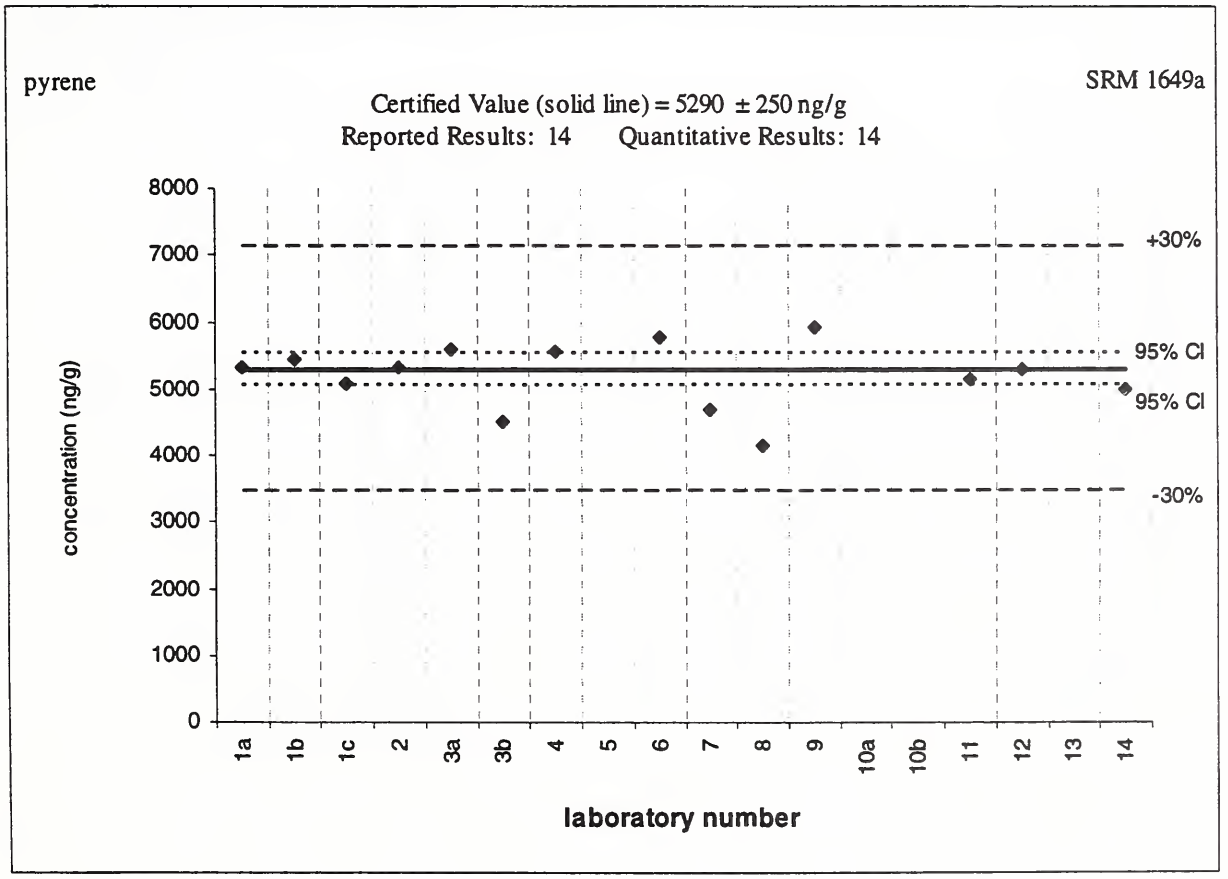
SRM 1649a

Certified Value (solid line) = 6450 ± 180 ng/g

Reported Results: 14 Quantitative Results: 14




pyrene
SRM 1648
Assigned value (solid line) = 6258 ng/g s = 647 ng/g 95% CL = 463 ng/g
Reported Results: 11 Quantitative Results: 11
concentration (ng/g)
12000
10000
8000
6000
4000
2000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

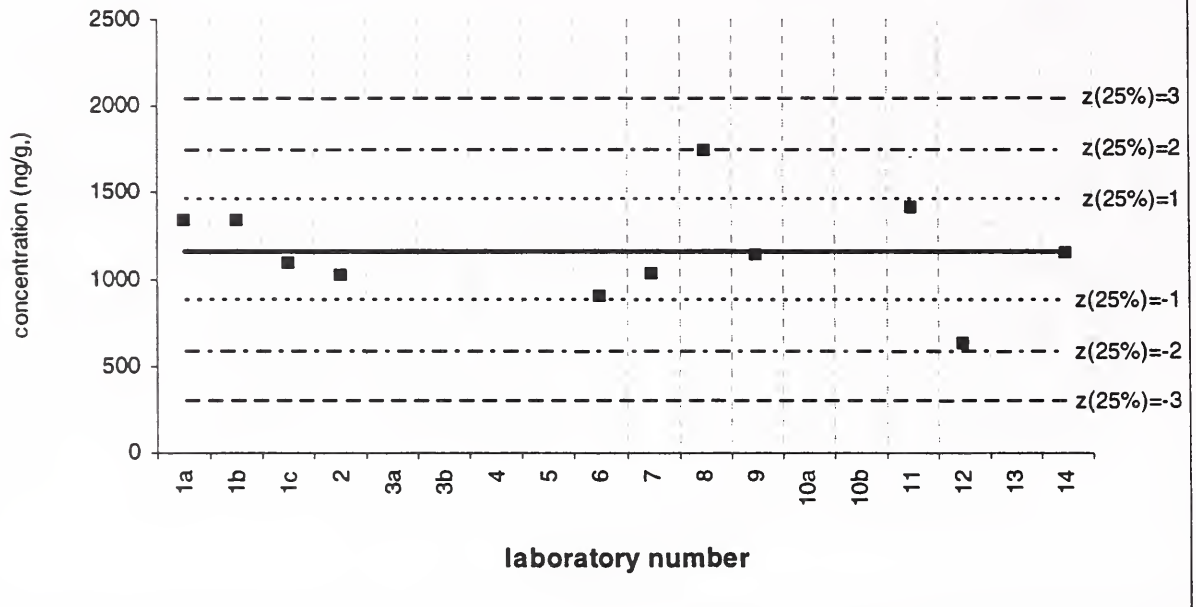

pyrene
SRM 1649a
Certified Value (solid line) = 5290 ± 250 ng/g
Reported Results: 14 Quantitative Results: 14
concentration (ng/g)
8000
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% CI
95% CI
-30%
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

pyrene

Baltimore 2 PM

Assigned value (solid line) = 1162 ng/g s = 294 ng/g 95% CL = 178 ng/g

Reported Results: 13 Quantitative Results: 13

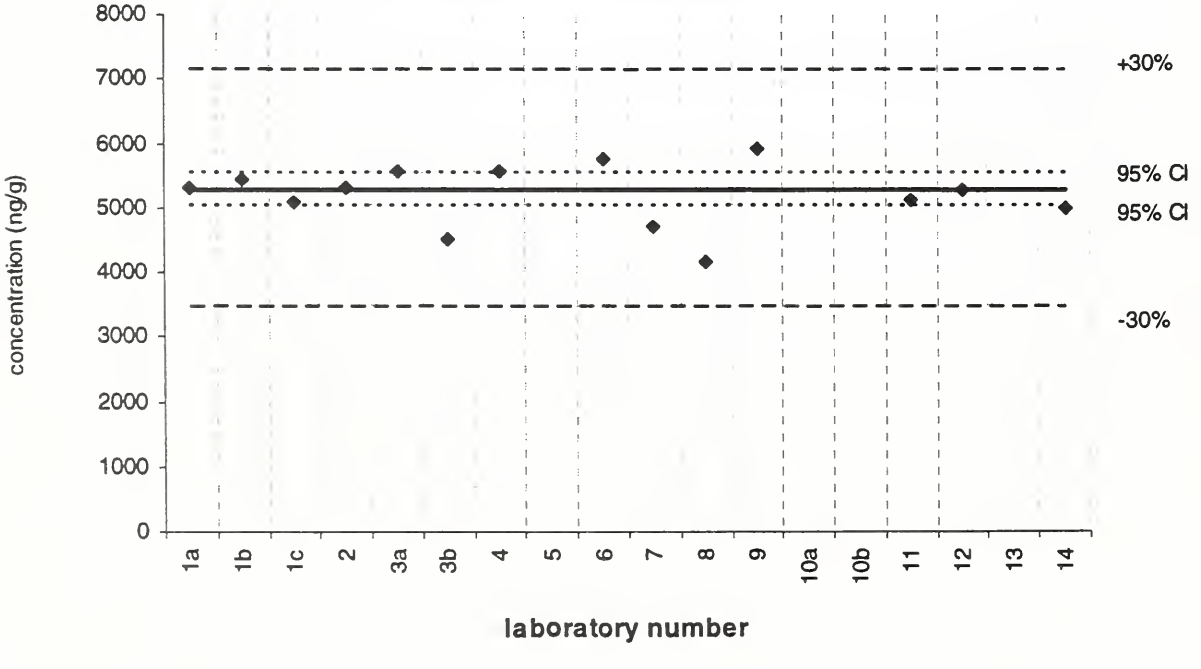


pyrene

SRM 1649a

Certified Value (solid line) = 5290 ± 250 ng/g

Reported Results: 14 Quantitative Results: 14

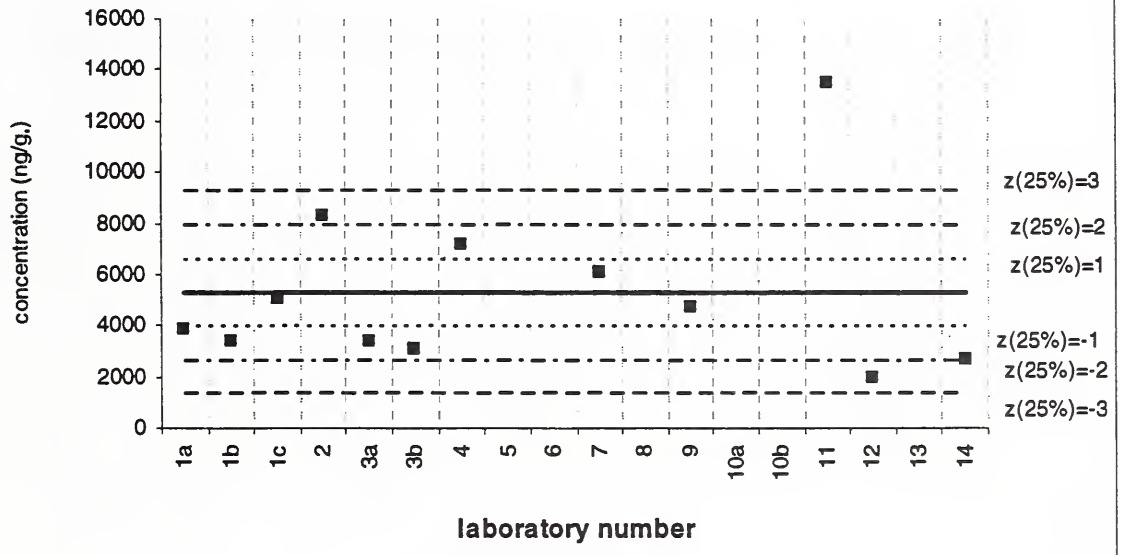


pyrene

Filter samples

Assigned value (solid line) = 5254 ng/g s = 3200 ng/g 95% CL = 2033 ng/g

Reported Results: 13 Quantitative Results: 12

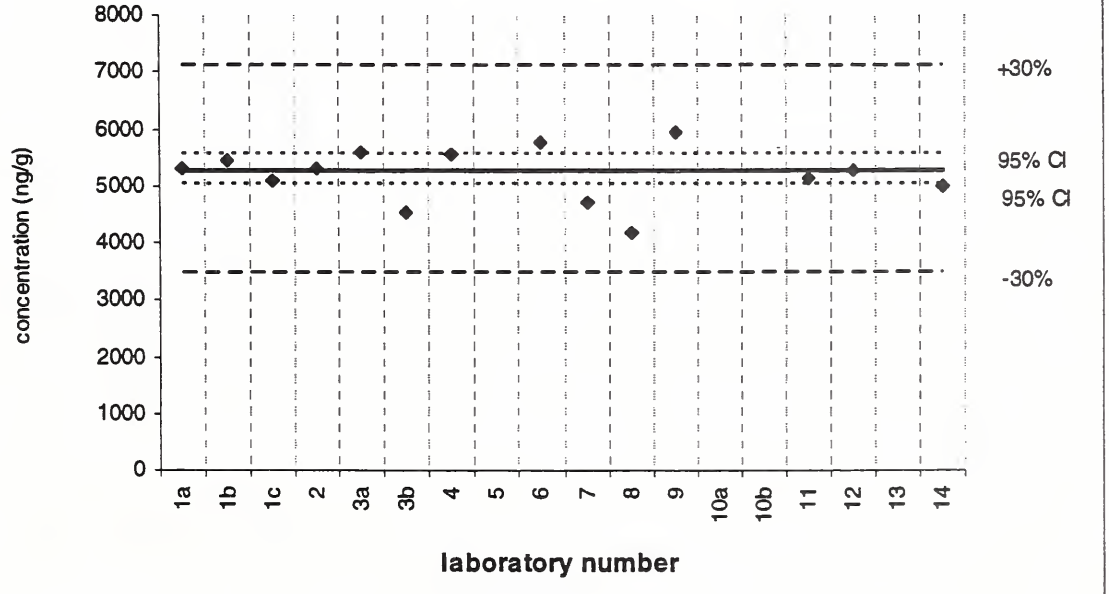


pyrene

SRM 1649a

Certified Value (solid line) = 5290 ± 250 ng/g

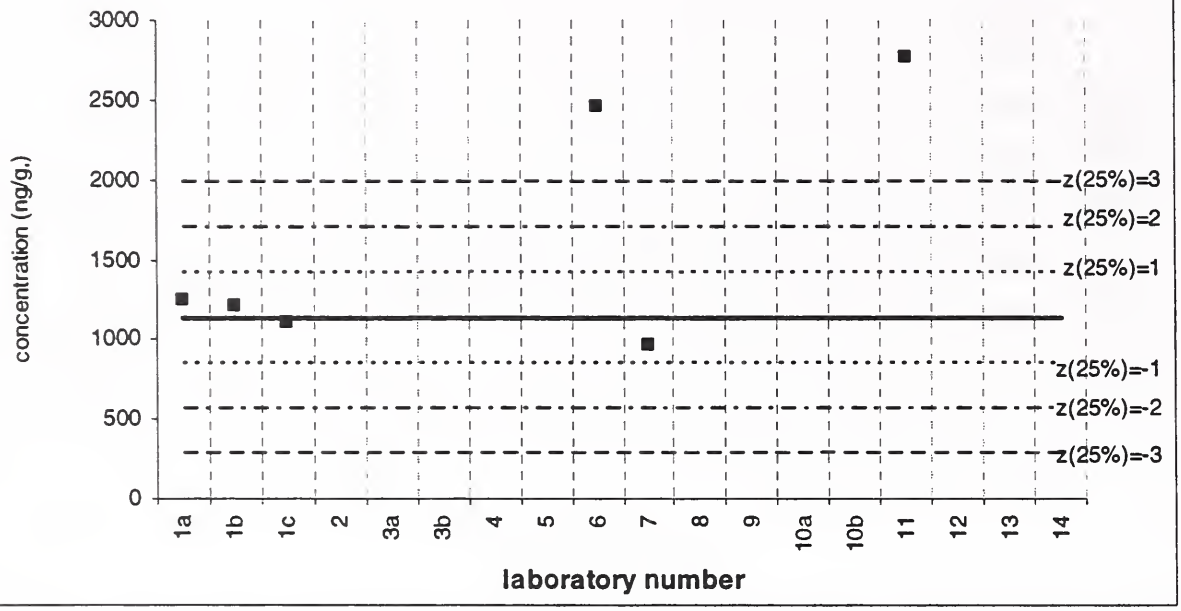
Reported Results: 14 Quantitative Results: 14



benzo[ghi]fluoranthene SRM 1648

Assigned value (solid line) = 1135 ng/g s = 124 ng/g 95% CL = 197 ng/g

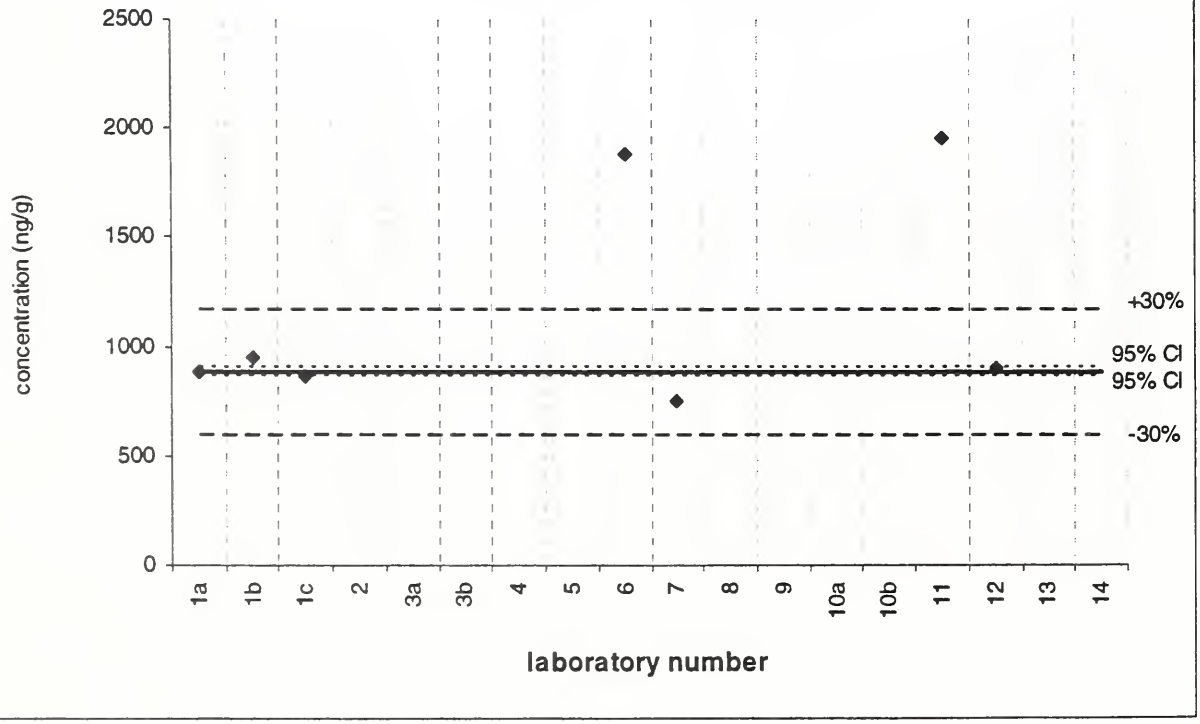
Reported Results: 7 Quantitative Results: 6



benzo[ghi]fluoranthene SRM 1649a

Reference Value (solid line) = 880 ± 20 ng/g

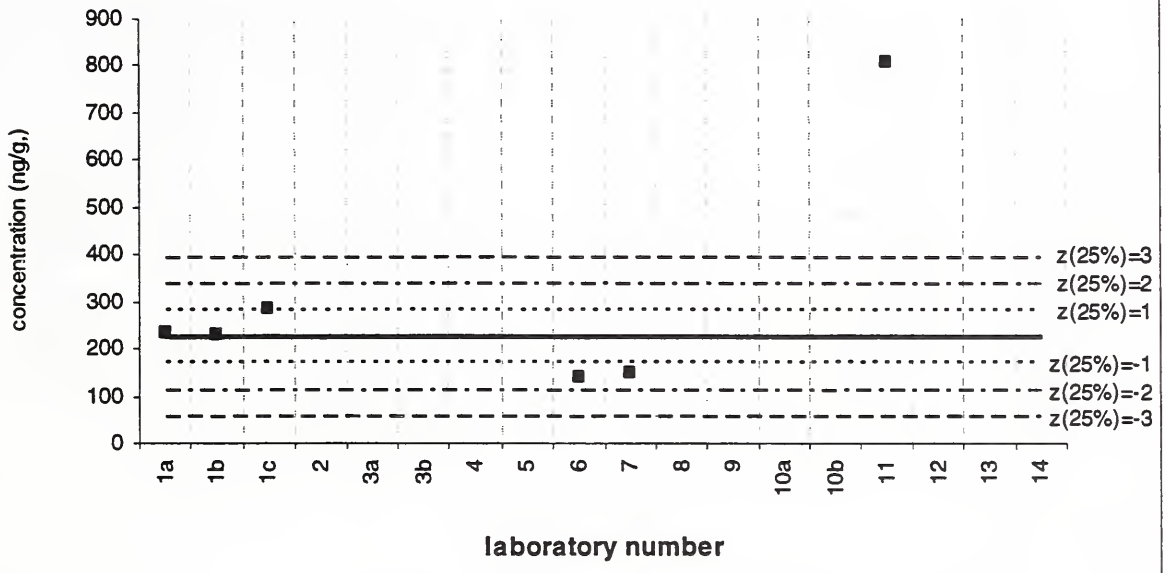
Reported Results: 7 Quantitative Results: 7



benzo[ghi]fluoranthene Baltimore 2 PM

Assigned value (solid line) = 225 ng/g s = 56 ng/g 95% CL = 90 ng/g

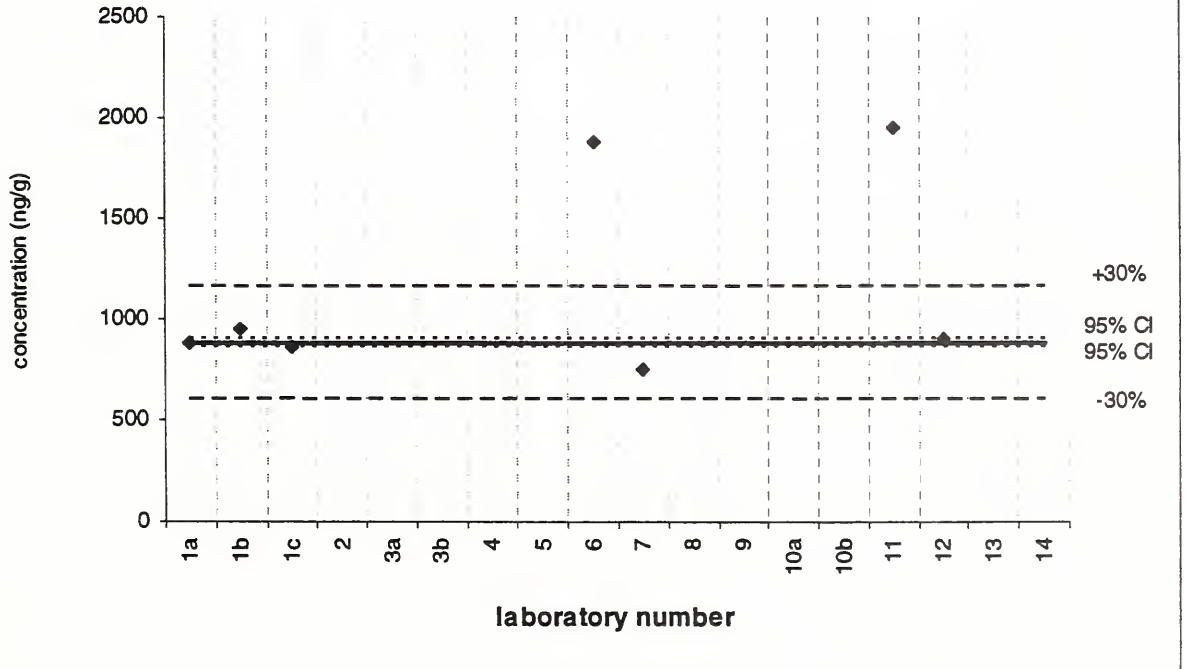
Reported Results: 7 Quantitative Results: 6



benzo[ghi]fluoranthene SRM 1649a

Reference Value (solid line) = 880 ± 20 ng/g

Reported Results: 7 Quantitative Results: 7



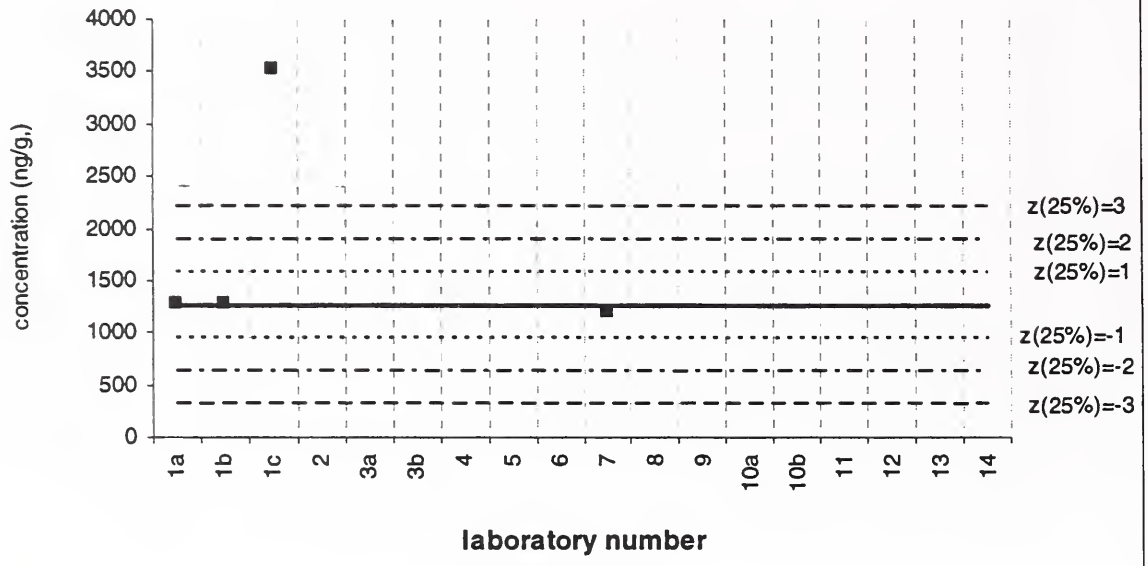
benzo[ghi]fluoranthene

Filter samples

Assigned value (solid line) = 1256 ng/g s = 48 ng/g 95% CL = 120 ng/g

Reported Results: 6 Quantitative Results: 5

Lab 11 = 13307 ng/g

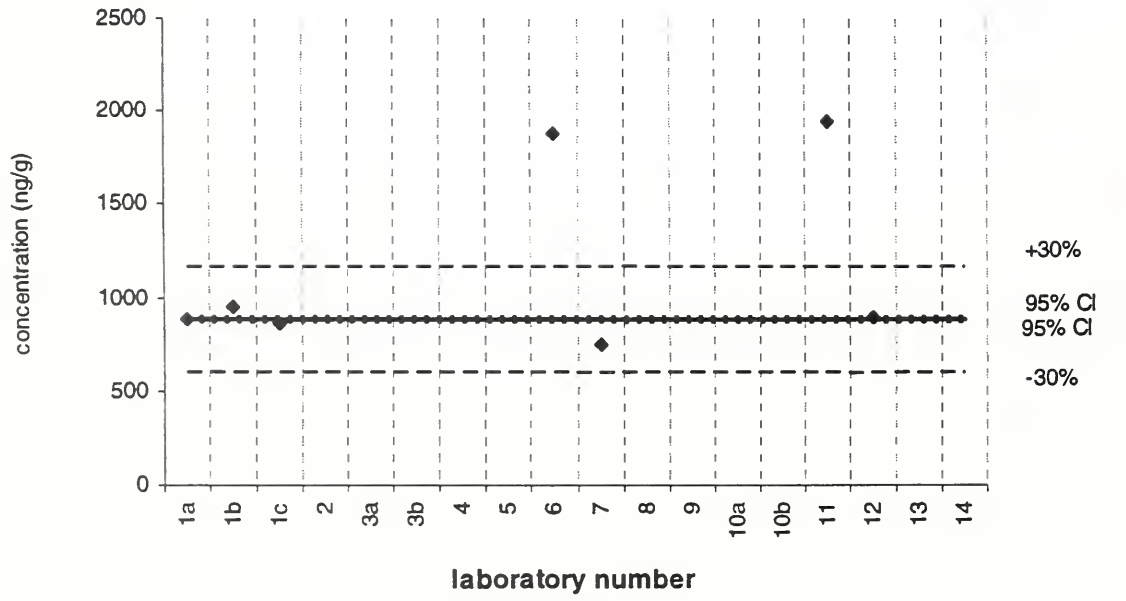


benzo[ghi]fluoranthene

SRM 1649a

Reference Value (solid line) = 880 ± 20 ng/g

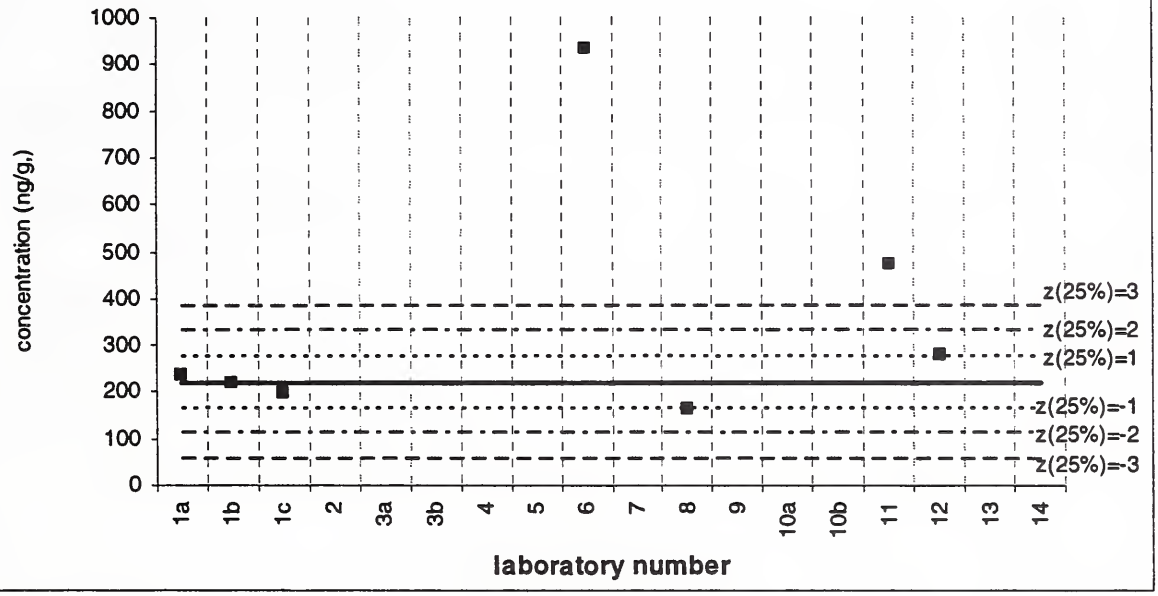
Reported Results: 7 Quantitative Results: 7



cyclopenta[cd]pyrene SRM 1648

Assigned value (solid line) = 219 ng/g s = 43 ng/g 95% CL = 53 ng/g

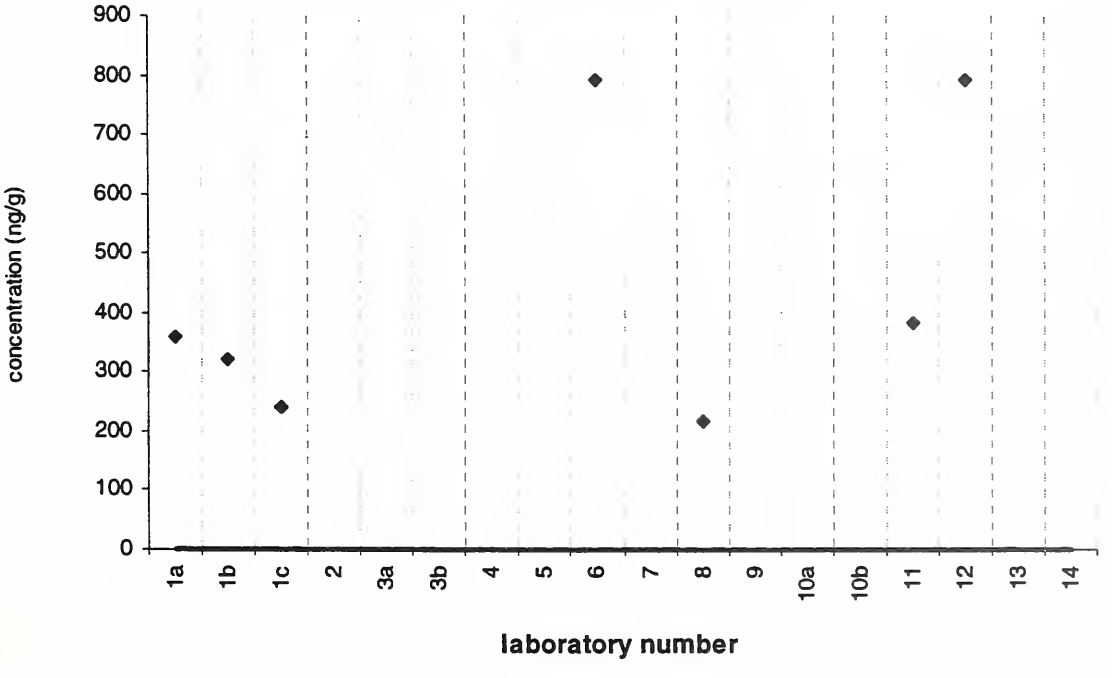
Reported Results: 7 Quantitative Results: 7



cyclopenta[cd]pyrene SRM 1649a

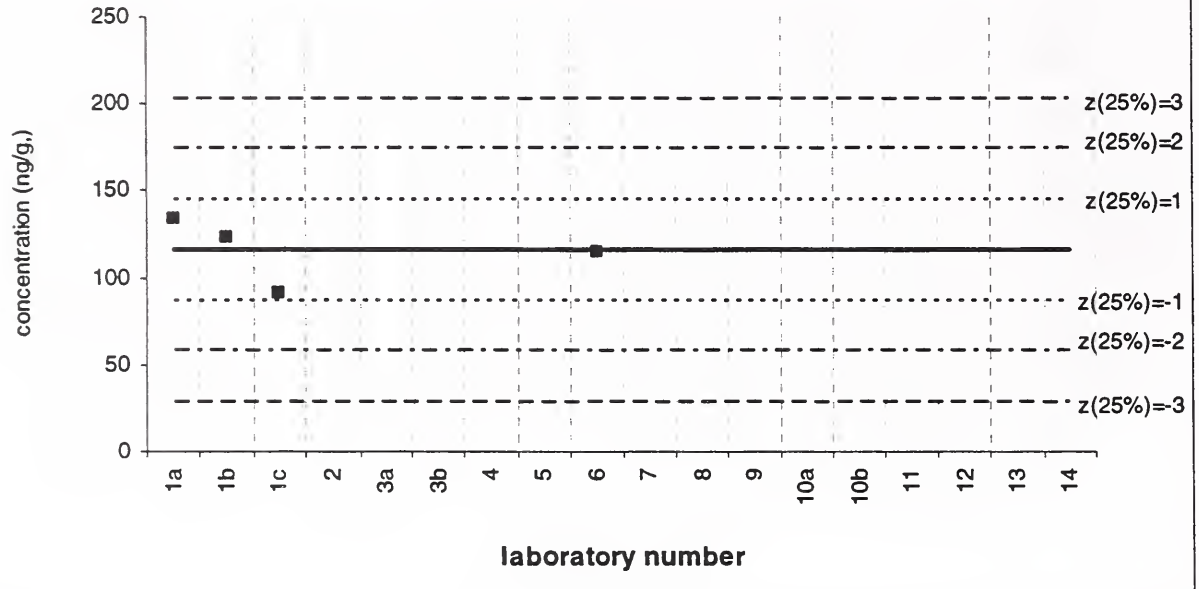
Target Value = no target ng/g

Reported Results: 7 Quantitative Results: 7



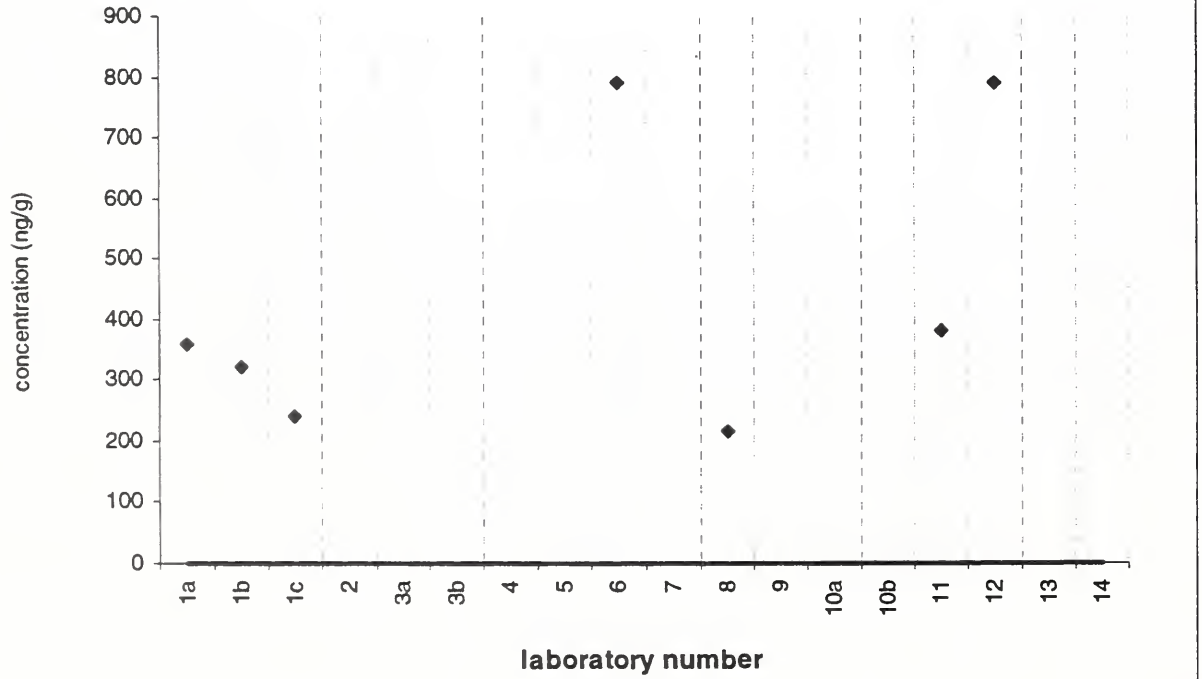
cyclopenta[cd]pyrene Baltimore 2 PM

Assigned value (solid line) = 116 ng/g s = 18 ng/g 95% CL = 28 ng/g
Reported Results: 7 Quantitative Results: 4



cyclopenta[cd]pyrene SRM 1649a

Target Value = no target ng/g
Reported Results: 7 Quantitative Results: 7

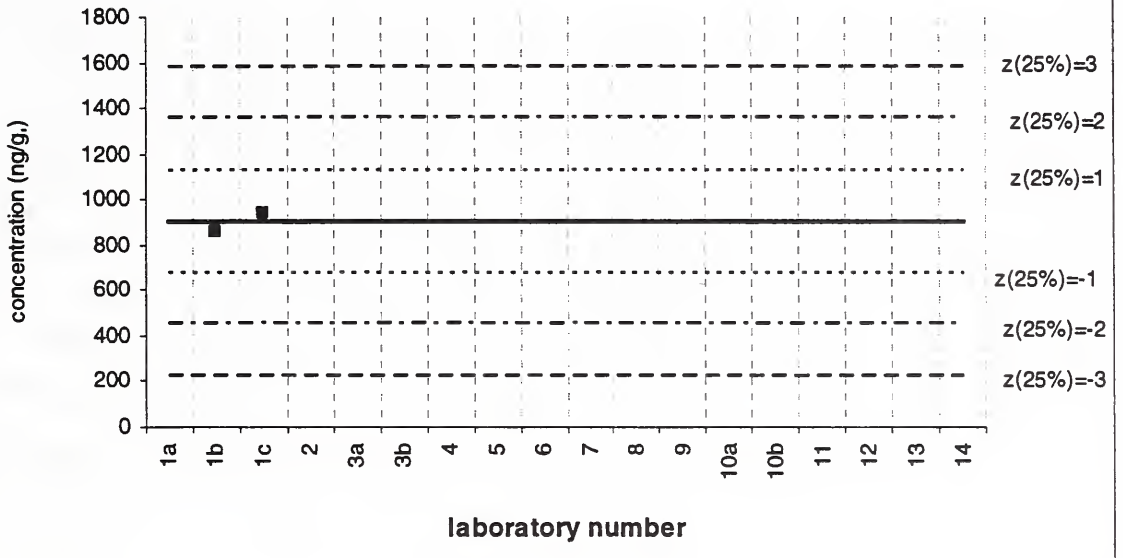


cyclopenta[cd]pyrene

Filter samples

Assigned value (solid line) = 902 ng/g s = 59 ng/g 95% CL = 533 ng/g

Reported Results: 6 Quantitative Results: 3



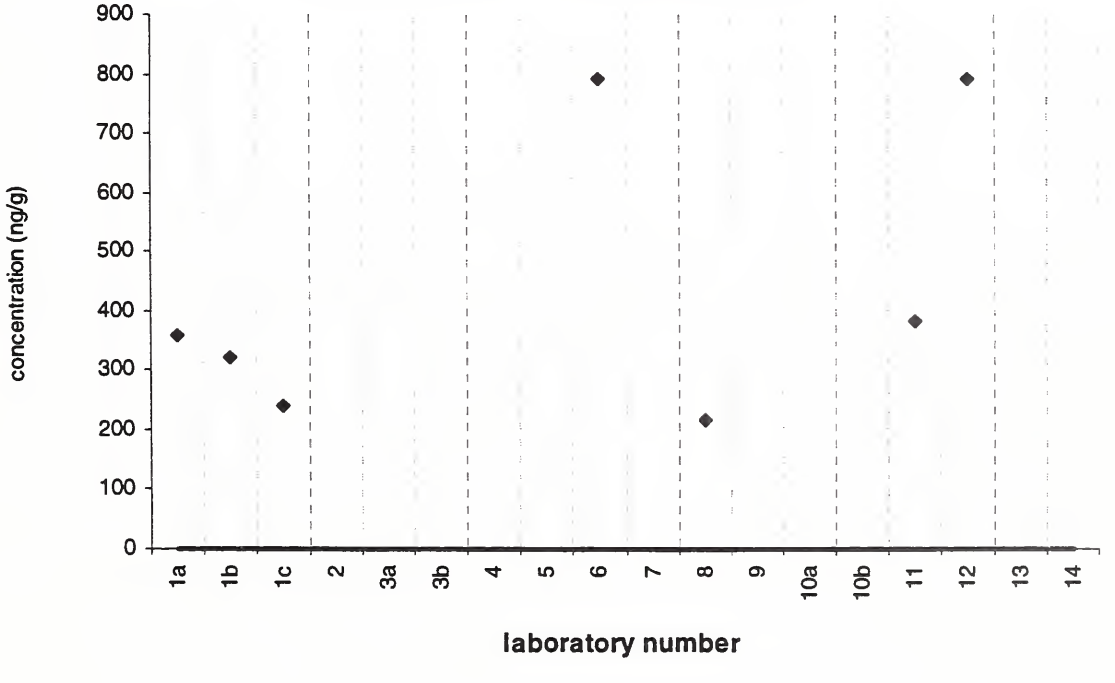
Lab 11 = 9390 ng/g

cyclopenta[cd]pyrene

SRM 1649a

Target Value = no target ng/g

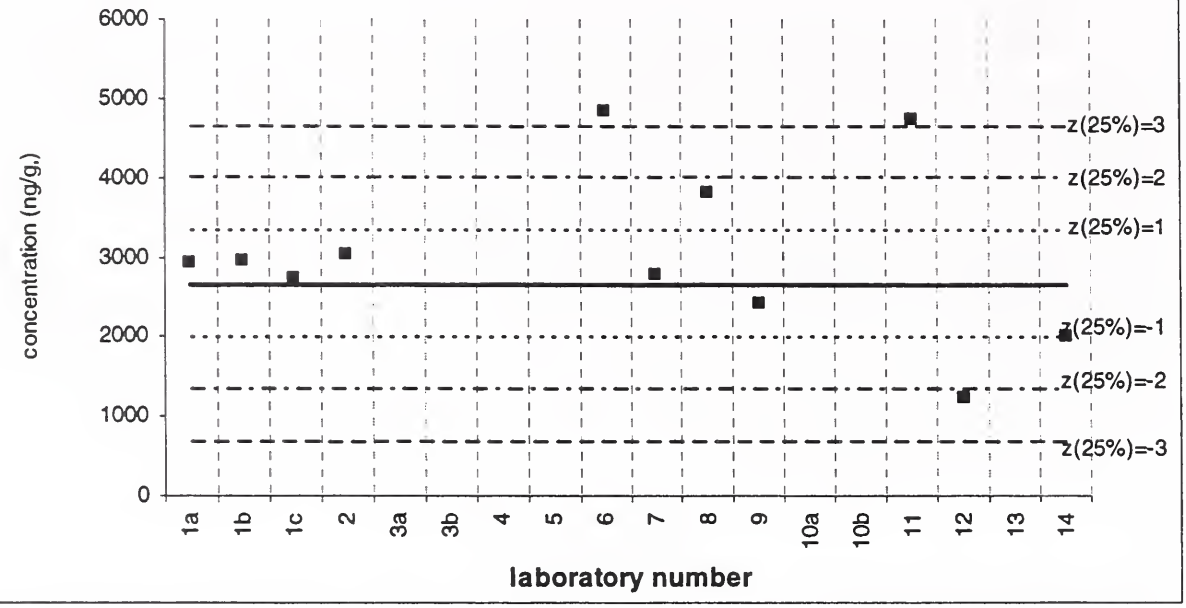
Reported Results: 7 Quantitative Results: 7



benz[a]anthracene

SRM 1648

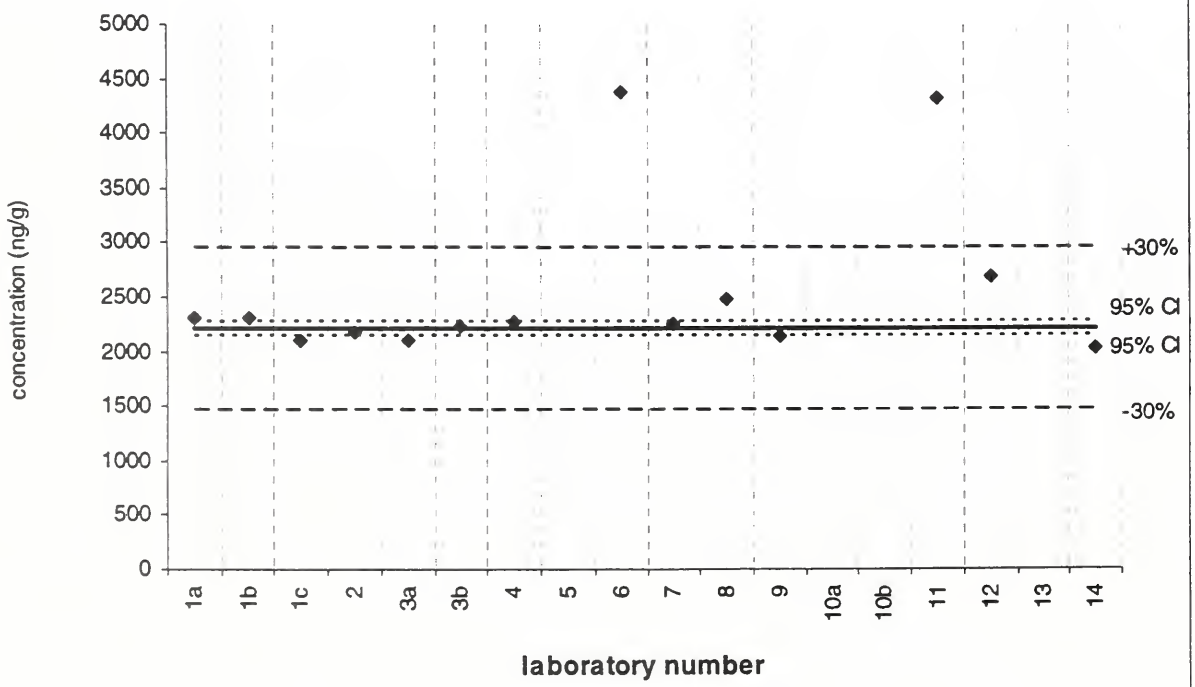
Assigned value (solid line) = 2654 ng/g s = 722 ng/g 95% CL = 555 ng/g
Reported Results: 11 Quantitative Results: 11



benz[a]anthracene

SRM 1649a

Certified Value (solid line) = 2210 ± 73 ng/g
Reported Results: 14 Quantitative Results: 14

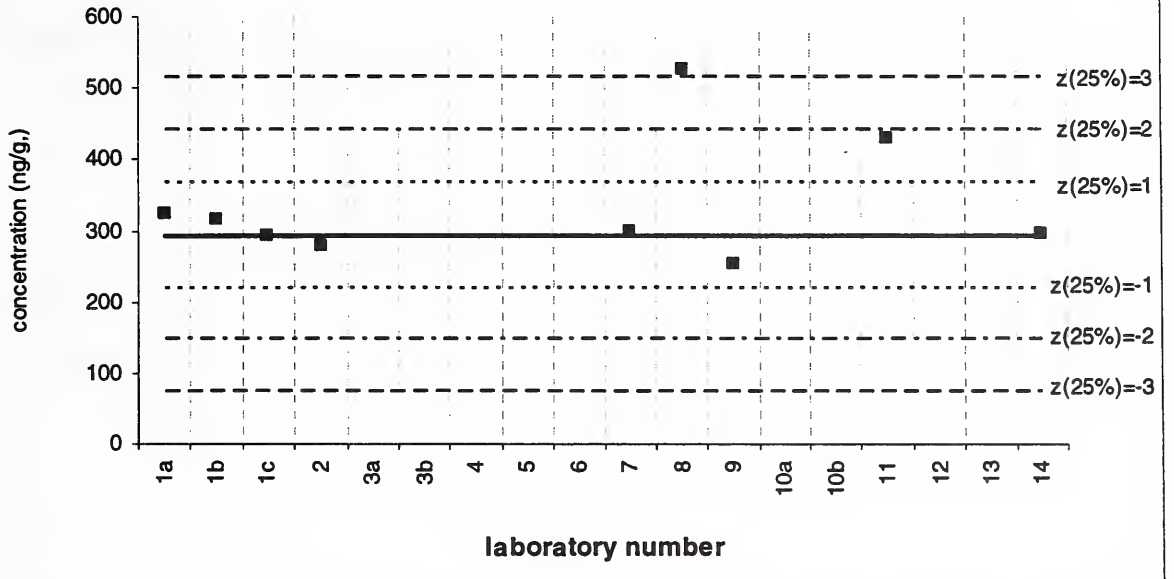


benz[a]anthracene

Baltimore 2 PM

Assigned value (solid line) = 294 ng/g s = 23 ng/g 95% CL = 22 ng/g

Reported Results: 11 Quantitative Results: 9

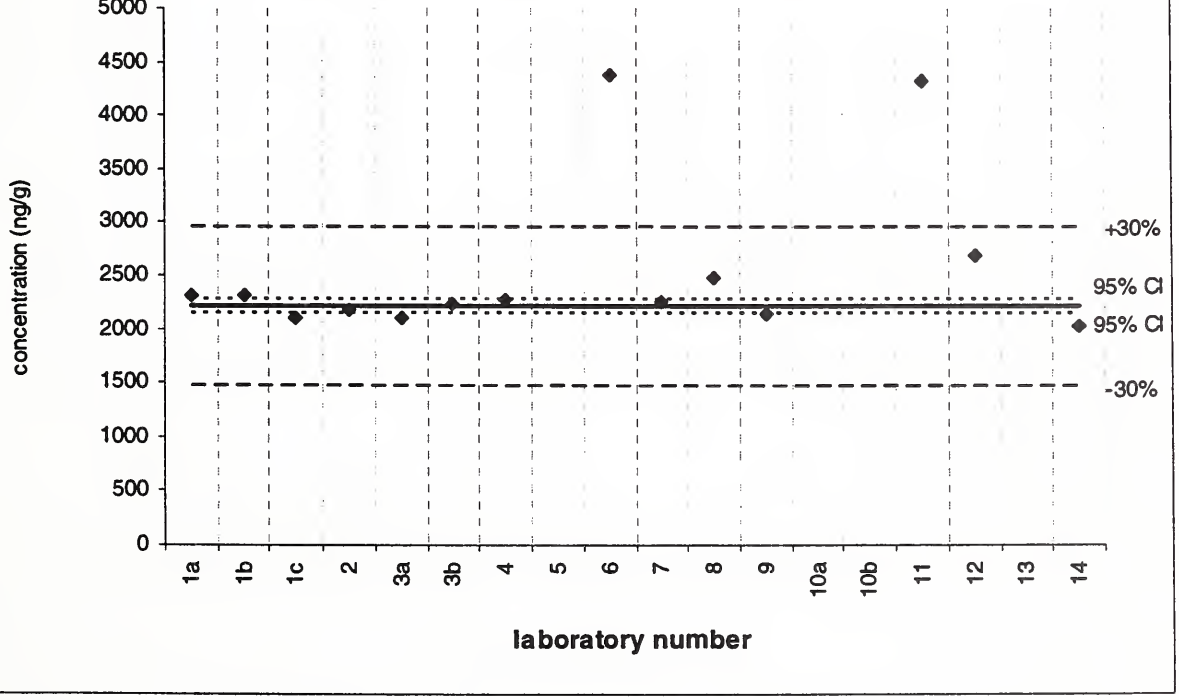


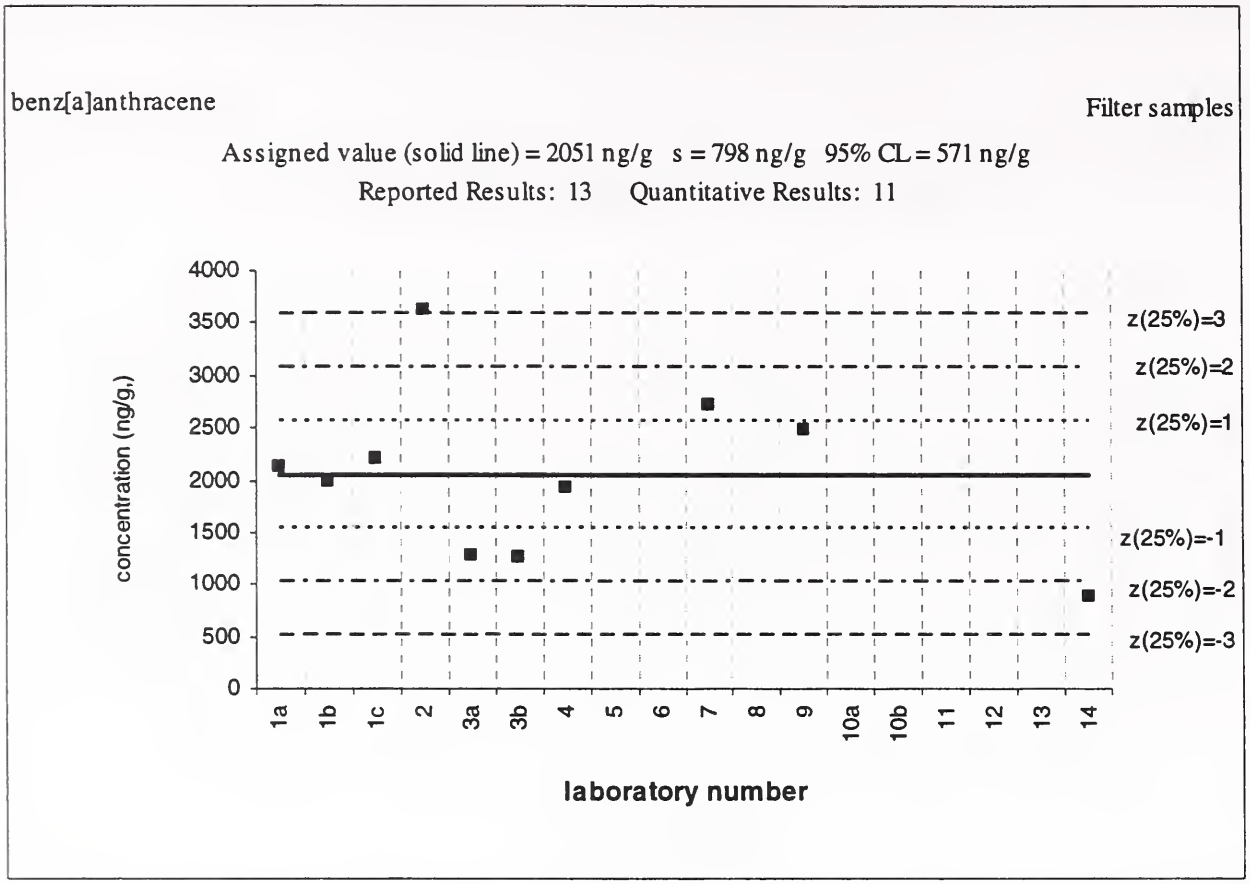
benz[a]anthracene

SRM 1649a

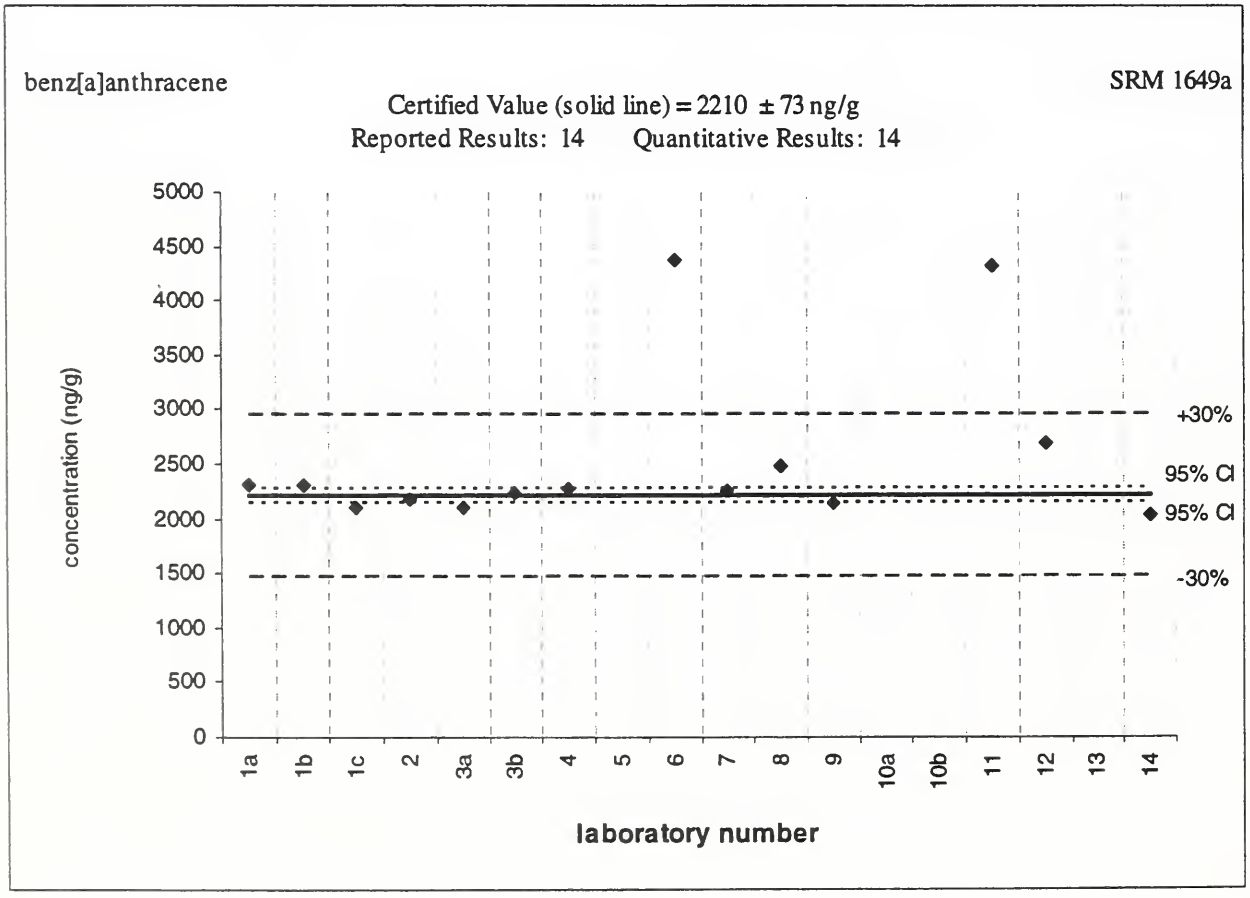
Certified Value (solid line) = 2210 ± 73 ng/g

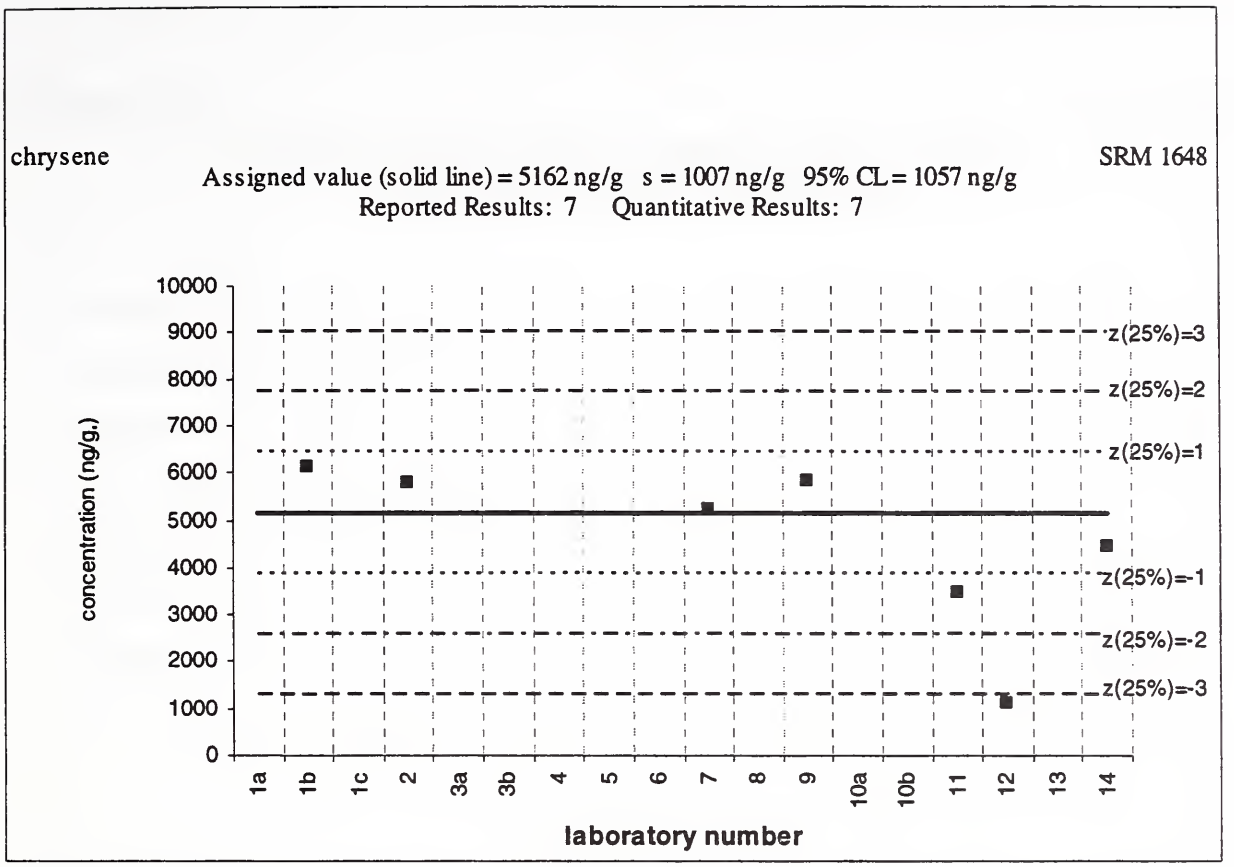
Reported Results: 14 Quantitative Results: 14

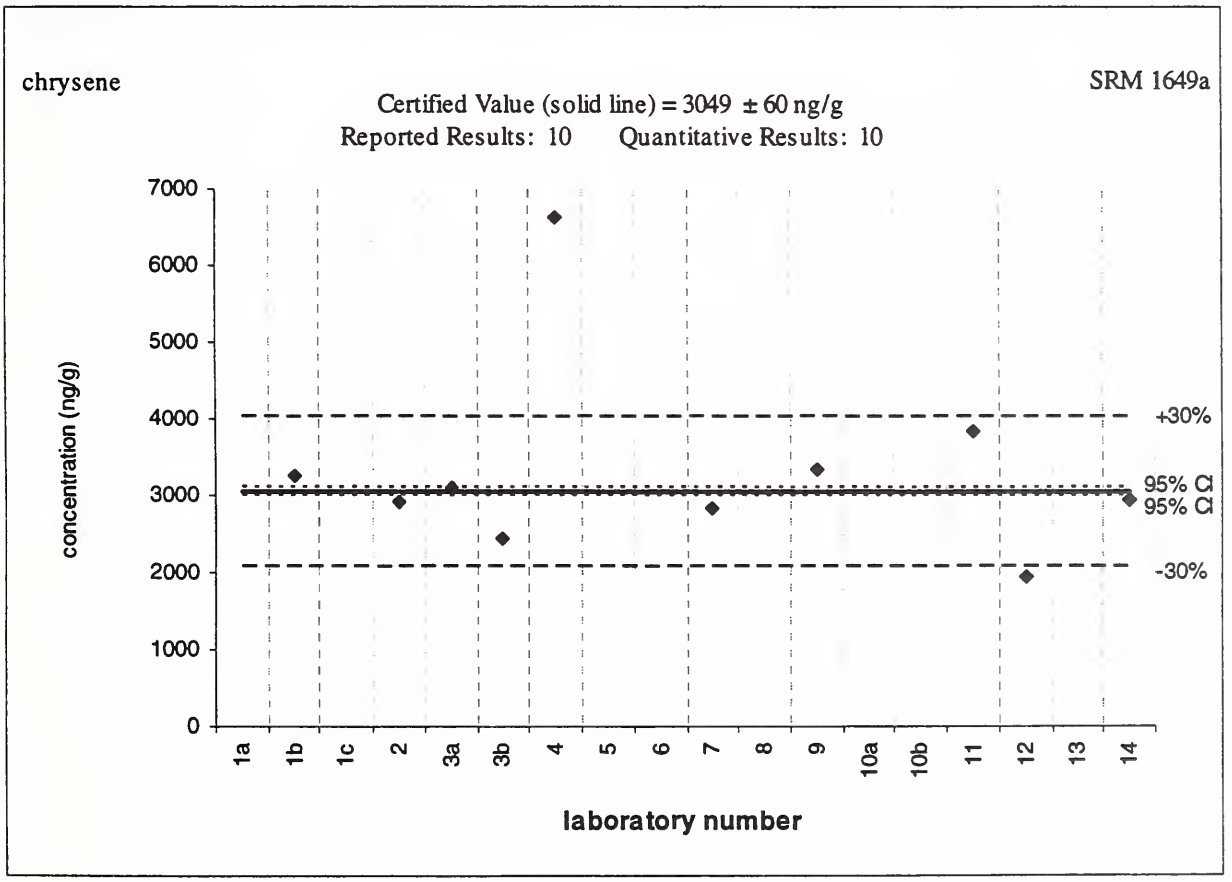


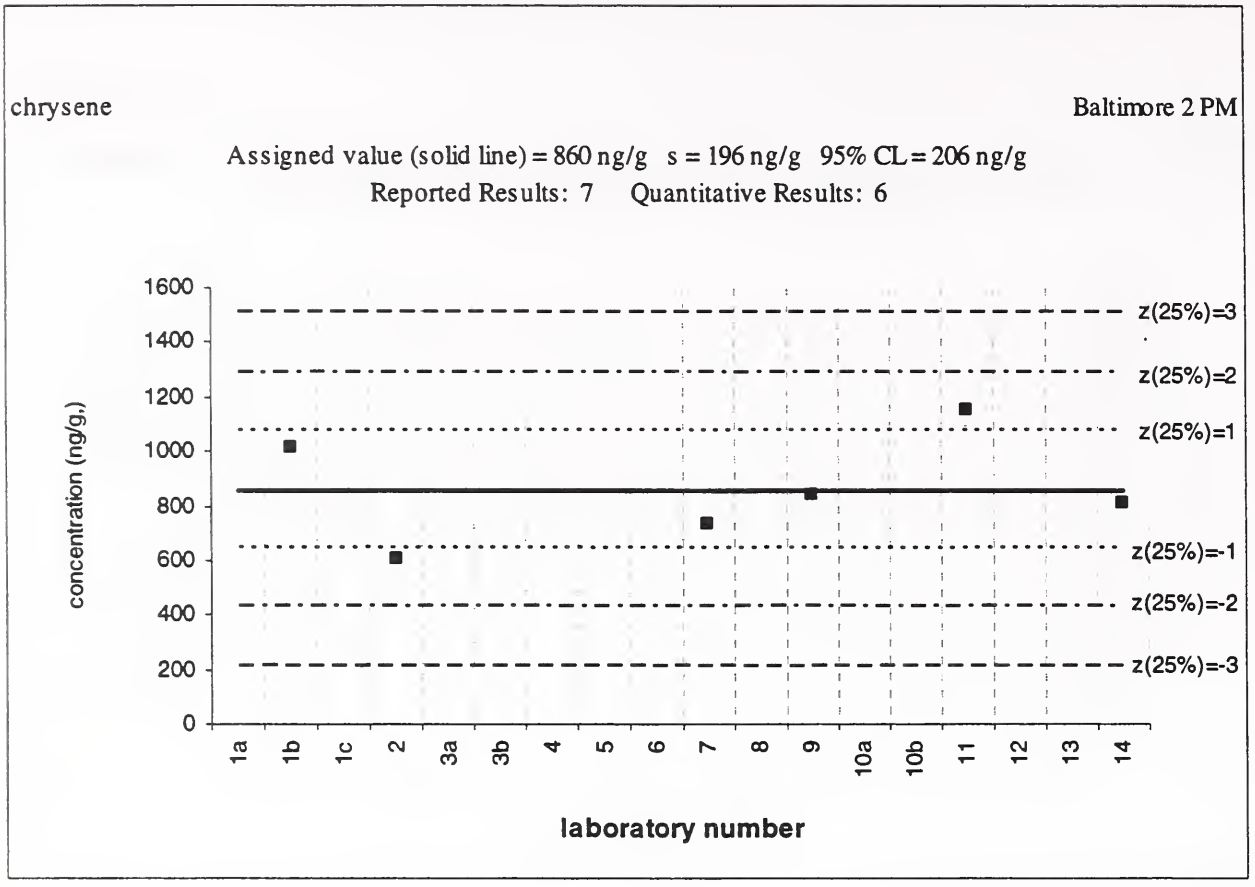


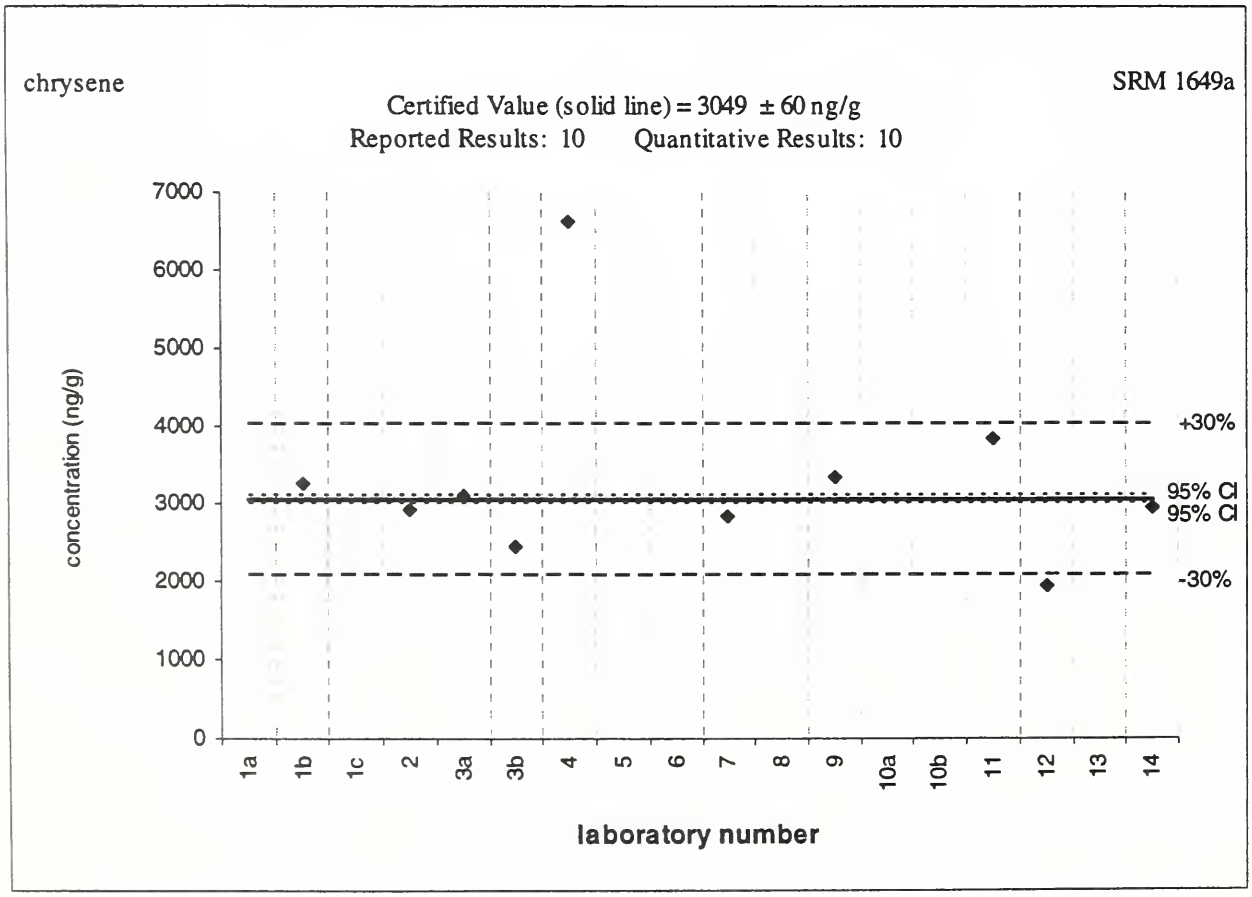
Lab 11 = 16518 ng/g

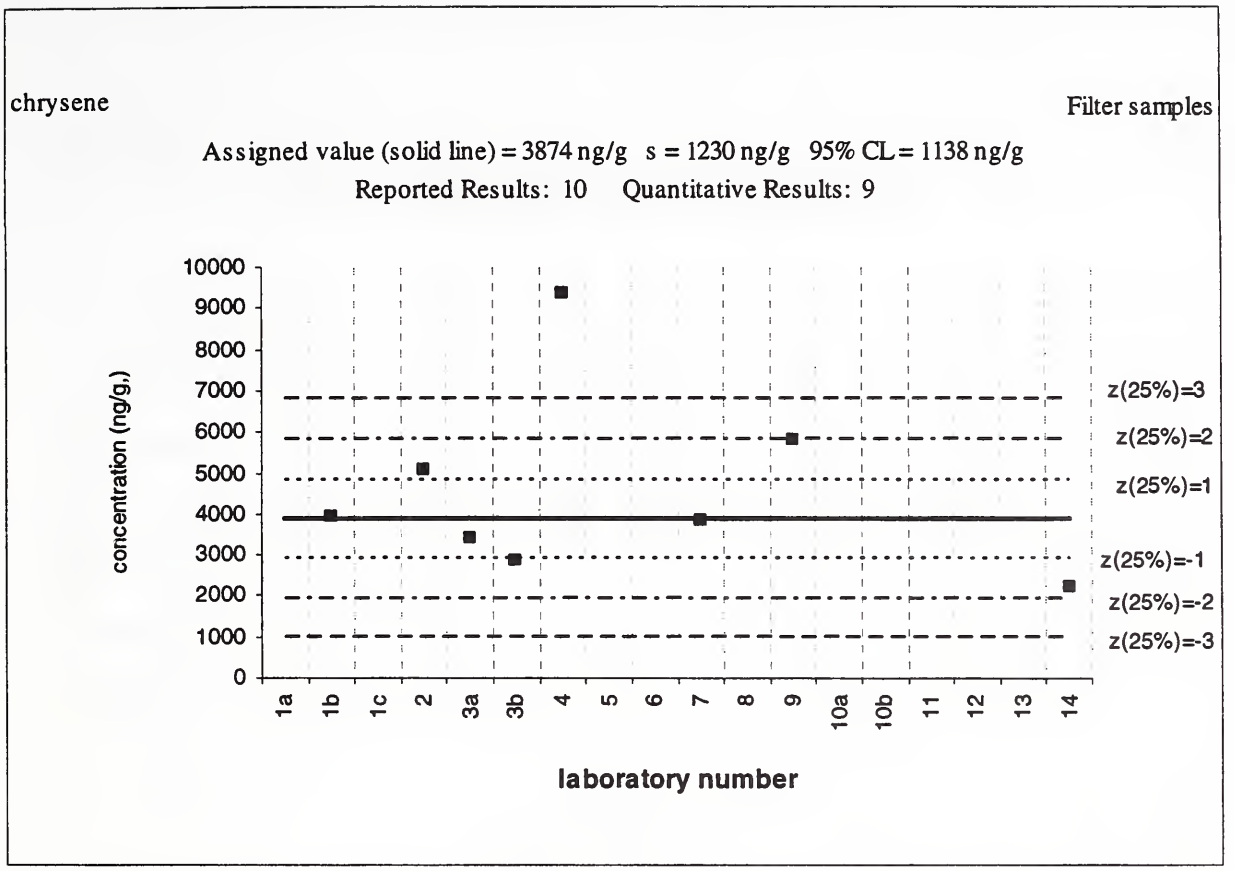



chrysene
SRM 1648
Assigned value (solid line) = 5162 ng/g s = 1007 ng/g 95% CL = 1057 ng/g
Reported Results: 7 Quantitative Results: 7
concentration (ng/g.)
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

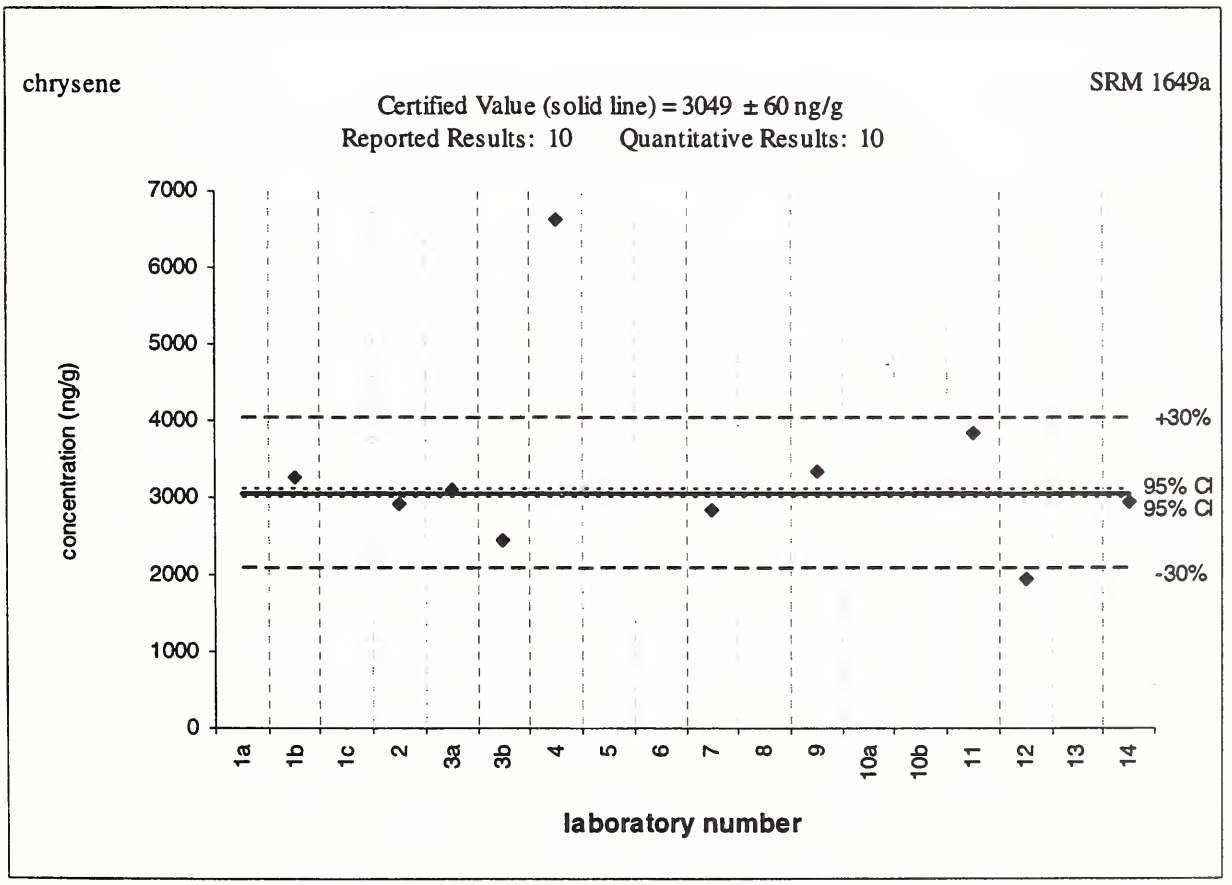

chrysene
SRM 1649a
Certified Value (solid line) = 3049 ± 60 ng/g
Reported Results: 10 Quantitative Results: 10
concentration (ng/g)
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% Ω
95% Ω
-30%
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

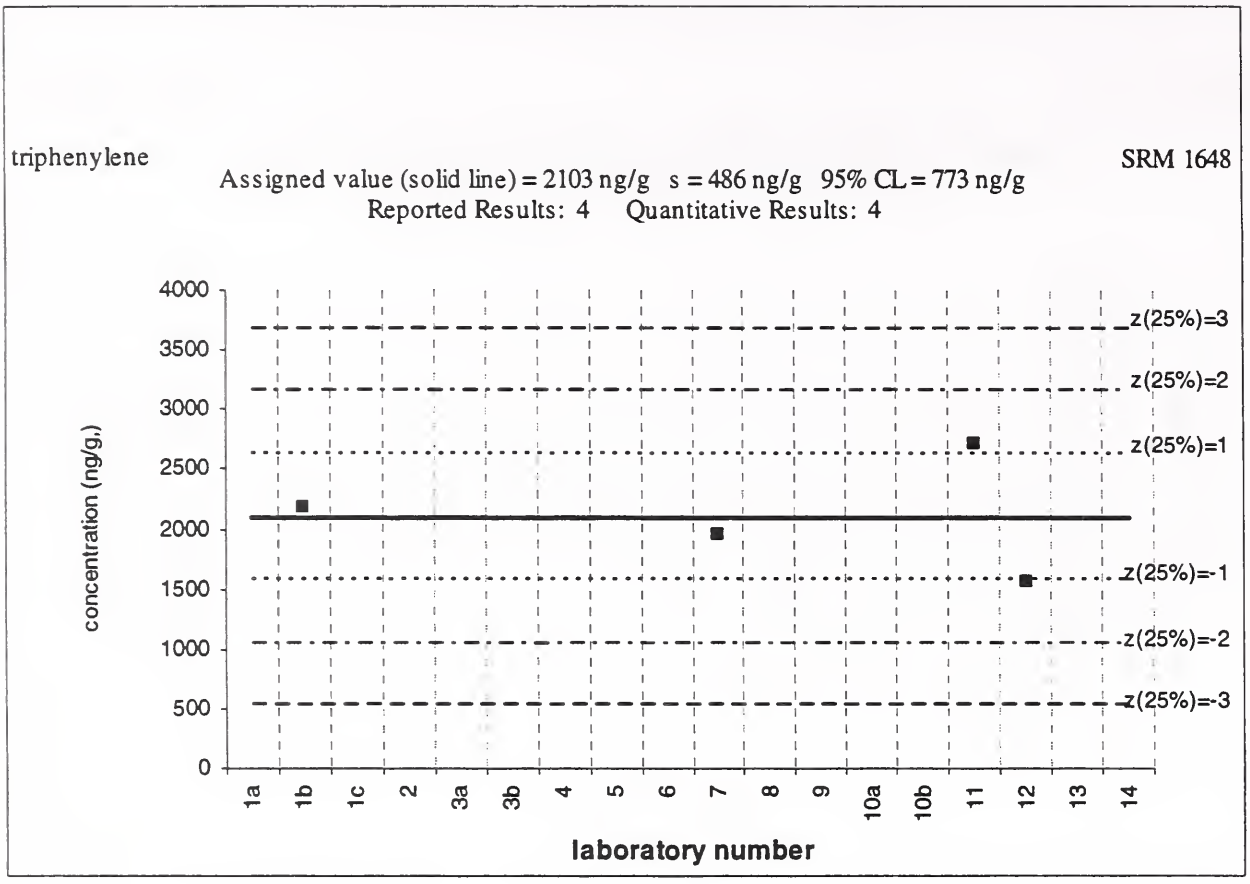

chrysene
Baltimore 2 PM
Assigned value (solid line) = 860 ng/g s = 196 ng/g 95% CL = 206 ng/g
Reported Results: 7 Quantitative Results: 6
concentration (ng/g.)
1600
1400
1200
1000
800
600
400
200
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

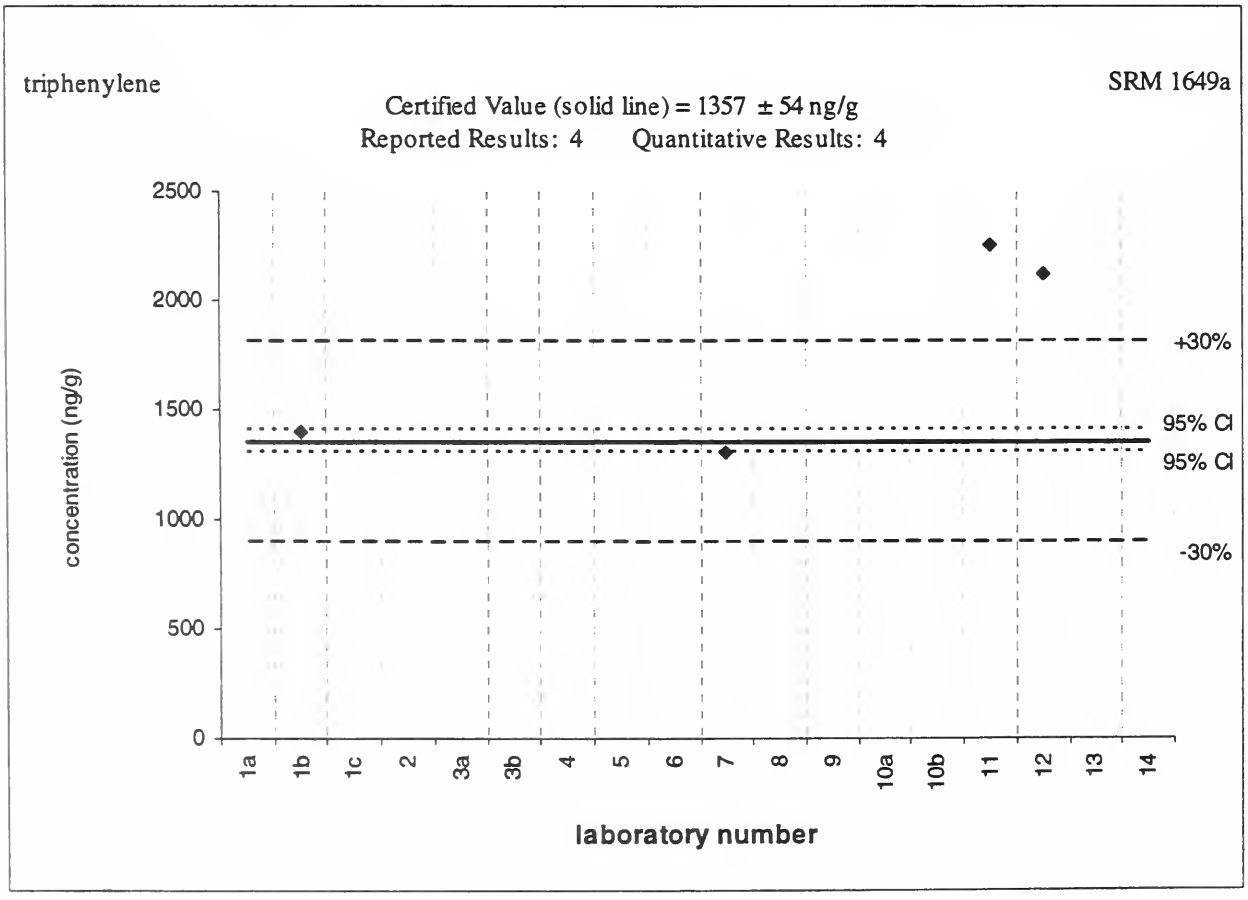

chrysene
SRM 1649a
Certified Value (solid line) = 3049 ± 60 ng/g
Reported Results: 10 Quantitative Results: 10
concentration (ng/g)
7000
6000
5000
4000
3000
2000
1000
0
+30%
95% CI
95% CI
-30%
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number



Lab 11 = 15907 ng/g




triphenylene
SRM 1648
Assigned value (solid line) = 2103 ng/g s = 486 ng/g 95% CL = 773 ng/g
Reported Results: 4 Quantitative Results: 4
concentration (ng/g,)
4000
3500
3000
2500
2000
1500
1000
500
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

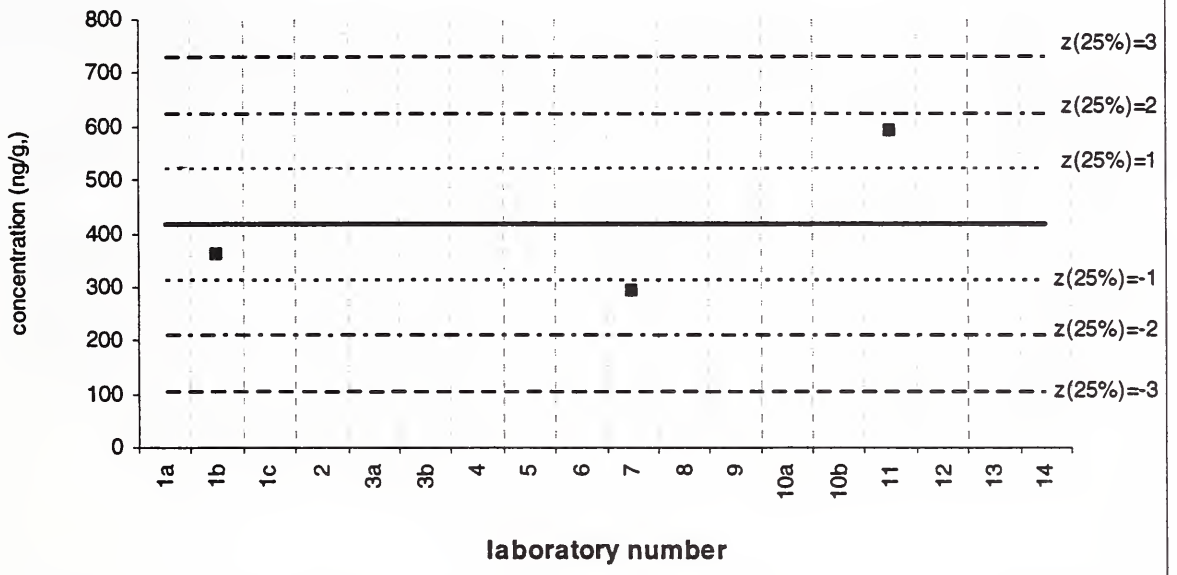

triphenylene
SRM 1649a
Certified Value (solid line) = 1357 ± 54 ng/g
Reported Results: 4 Quantitative Results: 4
concentration (ng/g)
2500
2000
1500
1000
500
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

triphenylene

Baltimore 2 PM

Assigned value (solid line) = 415 ng/g s = 158 ng/g 95% CL = 392 ng/g

Reported Results: 4 Quantitative Results: 3

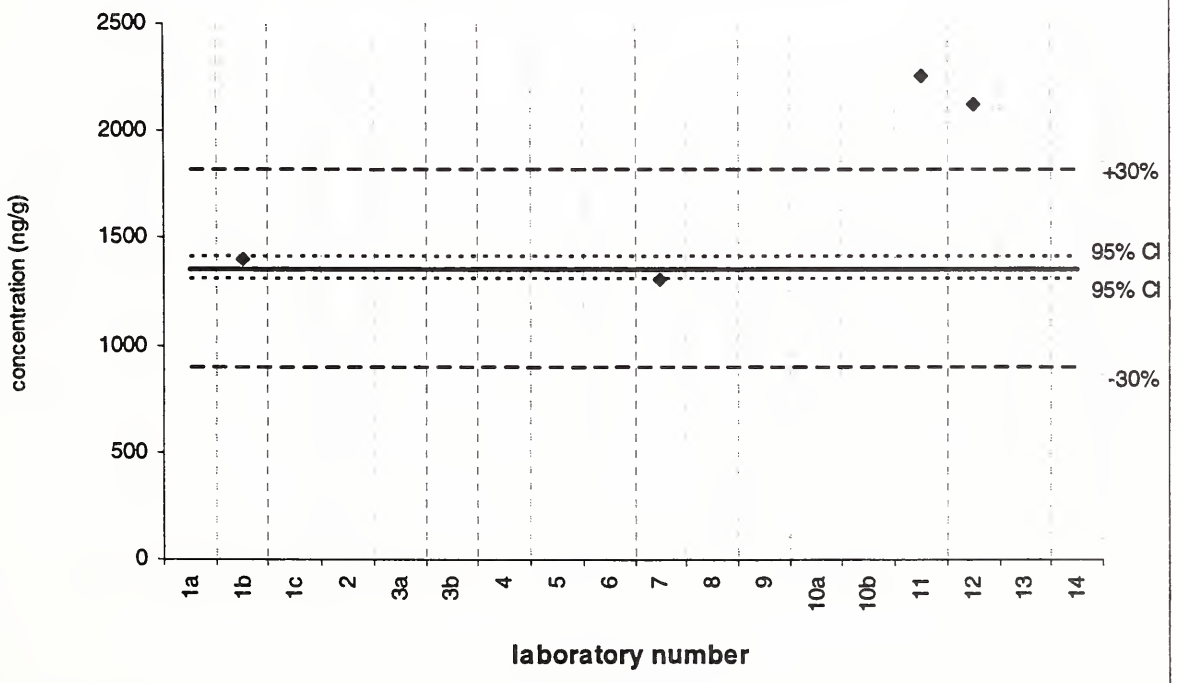


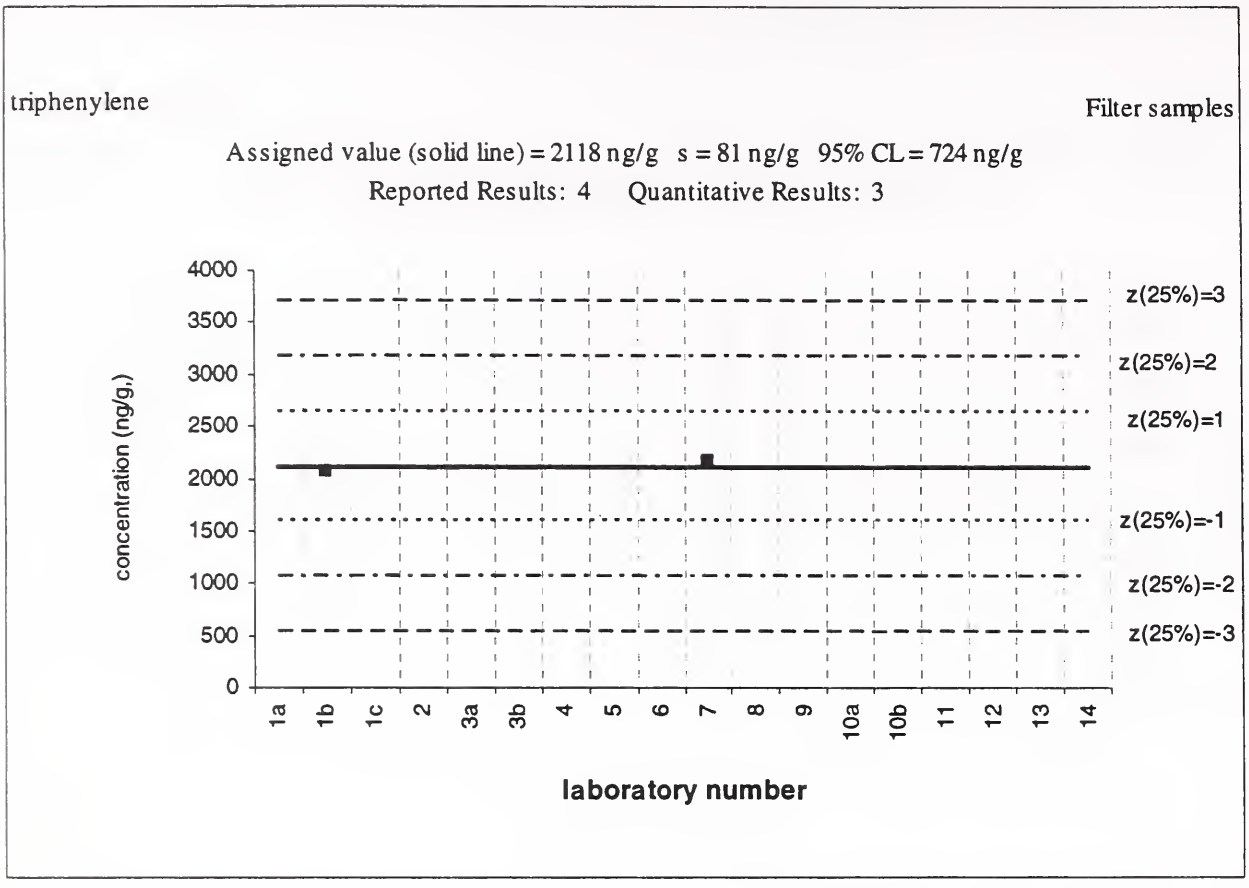
triphenylene

SRM 1649a

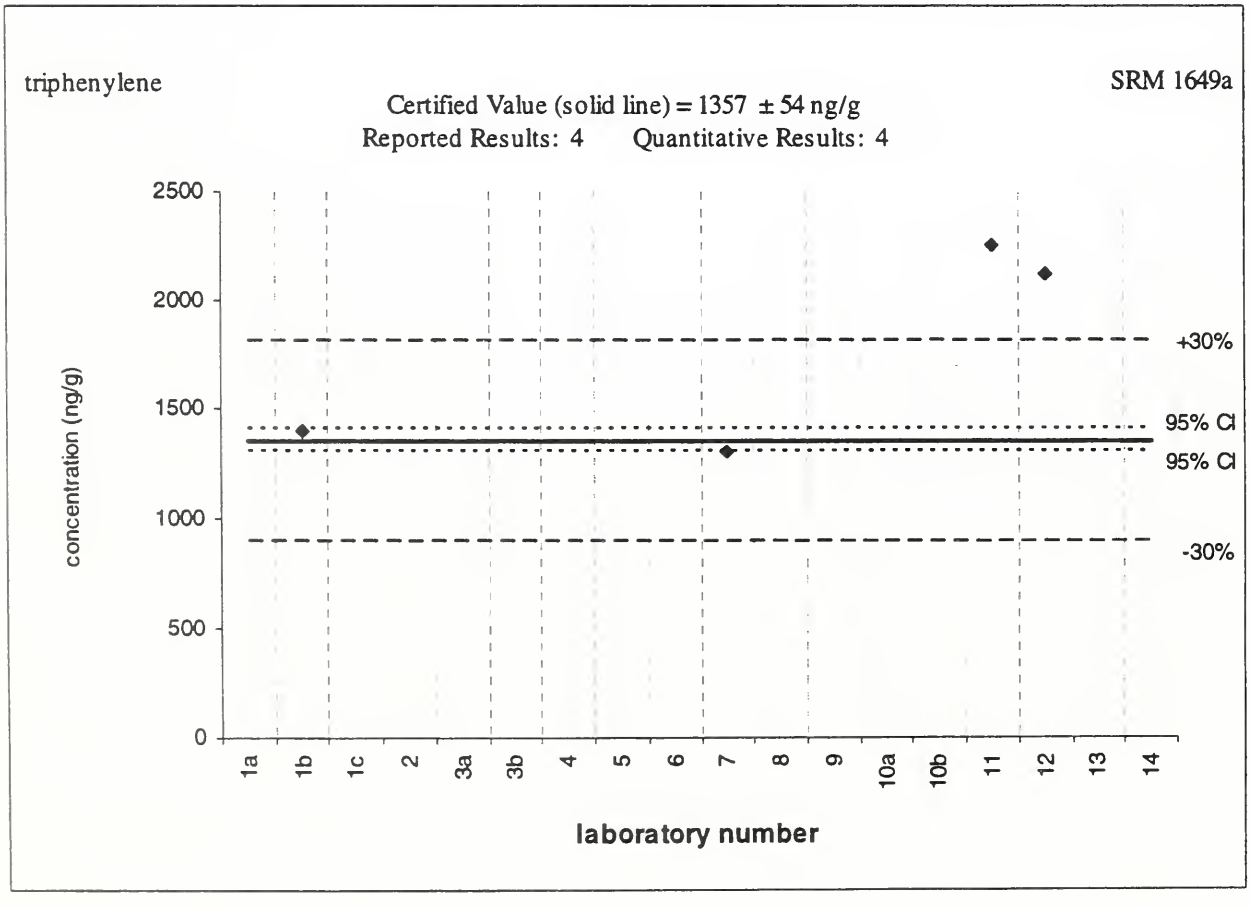
Certified Value (solid line) = 1357 ± 54 ng/g

Reported Results: 4 Quantitative Results: 4





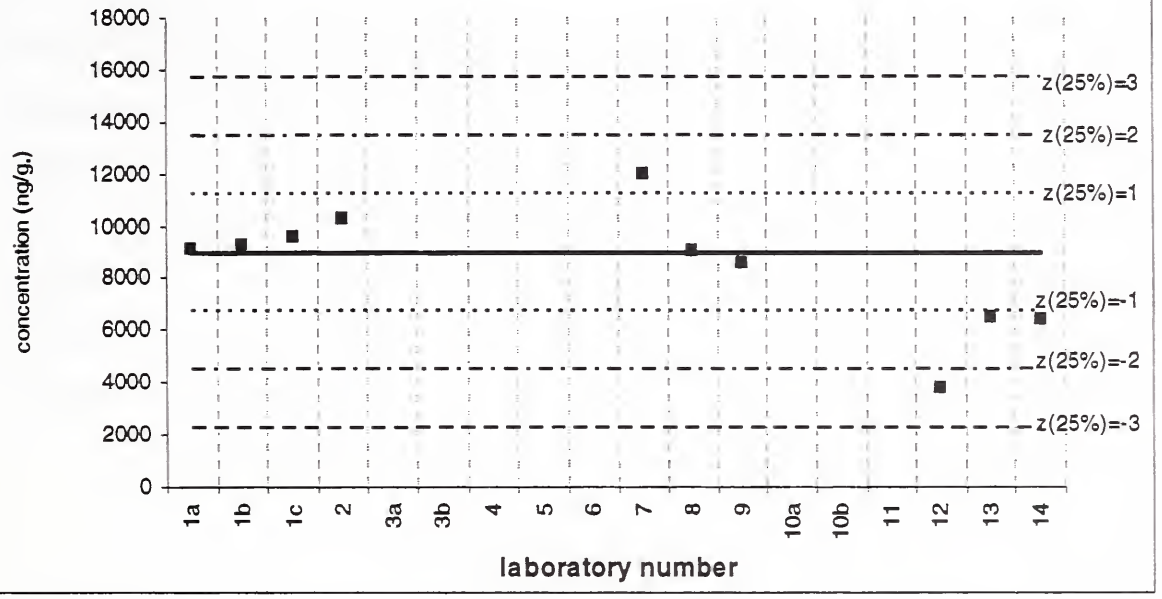
Lab 11 = 12515 ng/g



benzo[b]fluoranthene SRM 1648

Assigned value (solid line) = 8979 ng/g s = 1729 ng/g 95% CL = 1329 ng/g

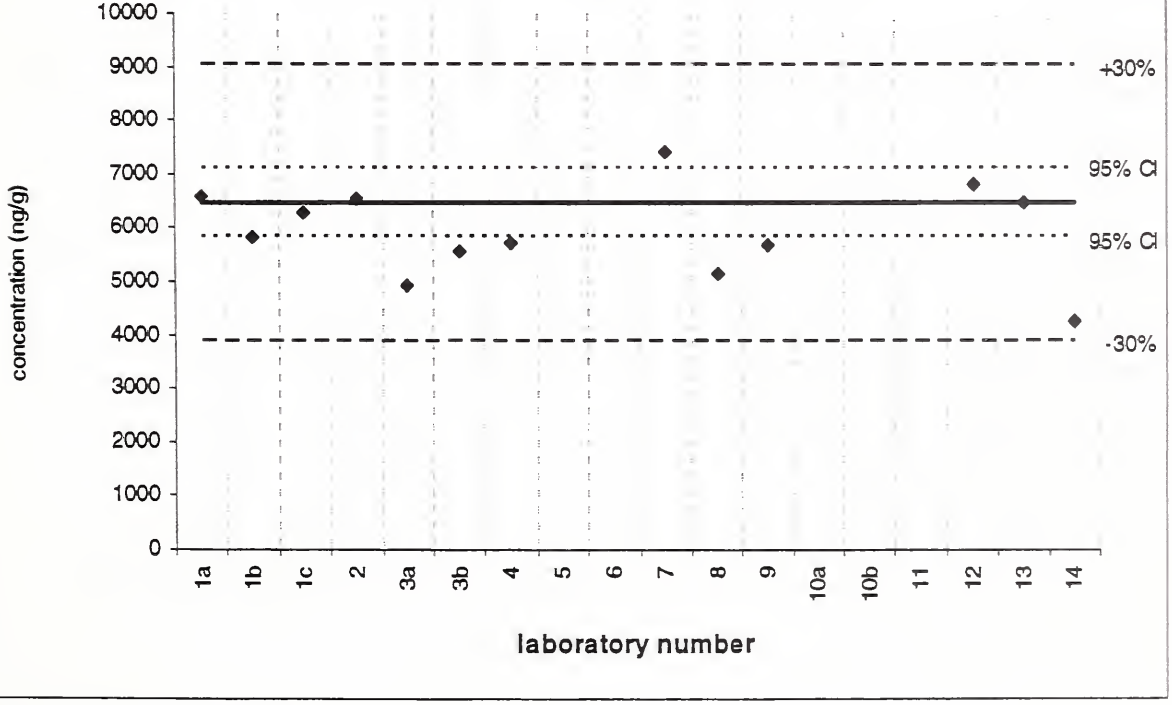
Reported Results: 10 Quantitative Results: 10



benzo[b]fluoranthene SRM 1649a

Certified Value (solid line) = 6450 ± 640 ng/g

Reported Results: 13 Quantitative Results: 13

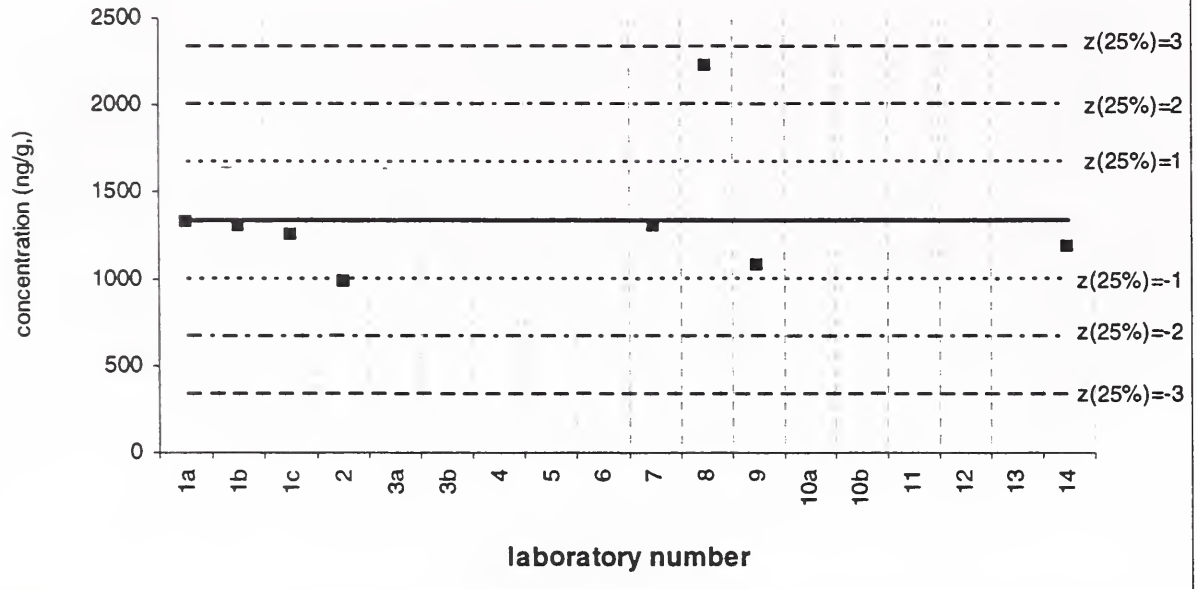


benzo[b]fluoranthene

Baltimore 2 PM

Assigned value (solid line) = 1334 ng/g s = 381 ng/g 95% CL = 319 ng/g

Reported Results: 9 Quantitative Results: 8

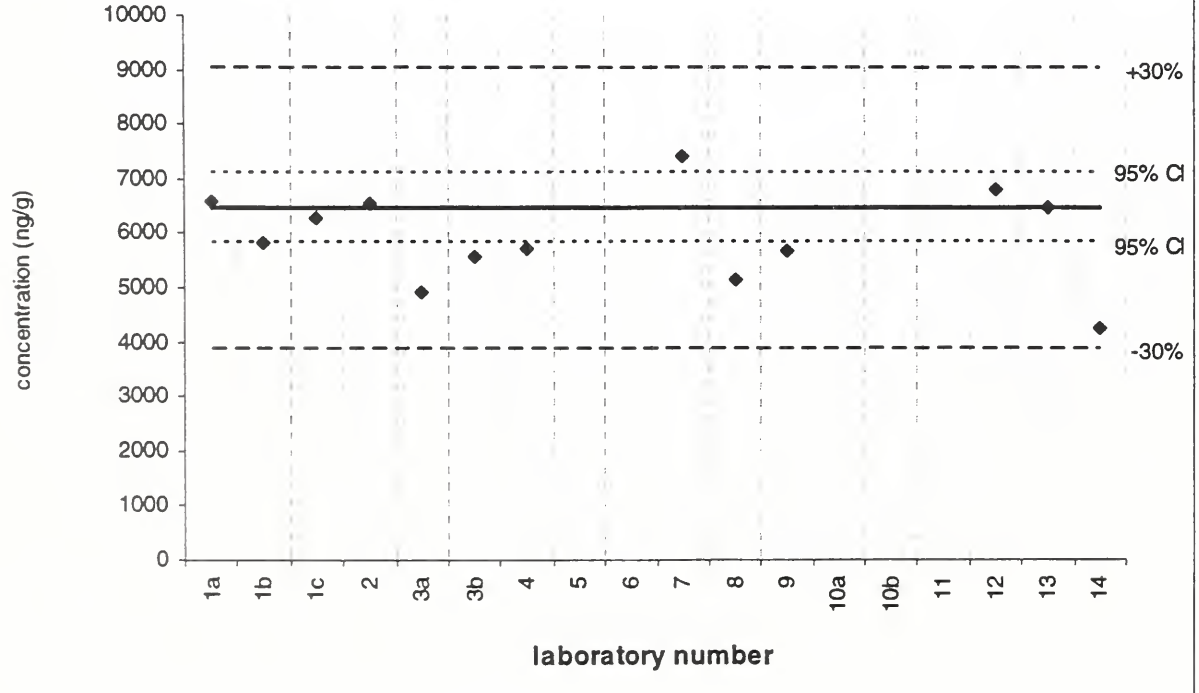


benzo[b]fluoranthene

SRM 1649a

Certified Value (solid line) = 6450 ± 640 ng/g

Reported Results: 13 Quantitative Results: 13

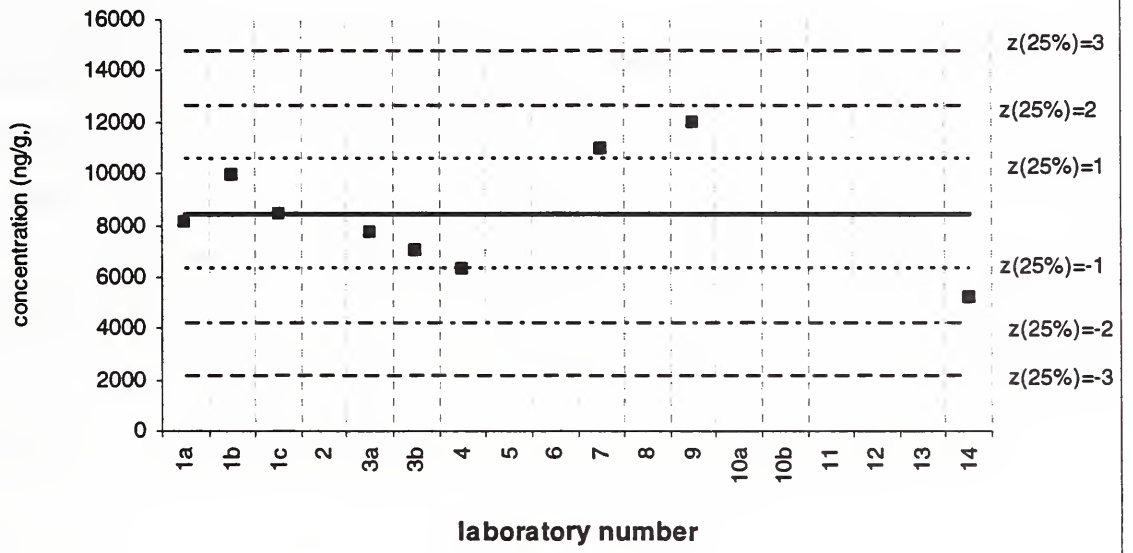


benzo[b]fluoranthene

Filter samples

Assigned value (solid line) = 8424 ng/g s = 2202 ng/g 95% CL = 1692 ng/g

Reported Results: 11 Quantitative Results: 9

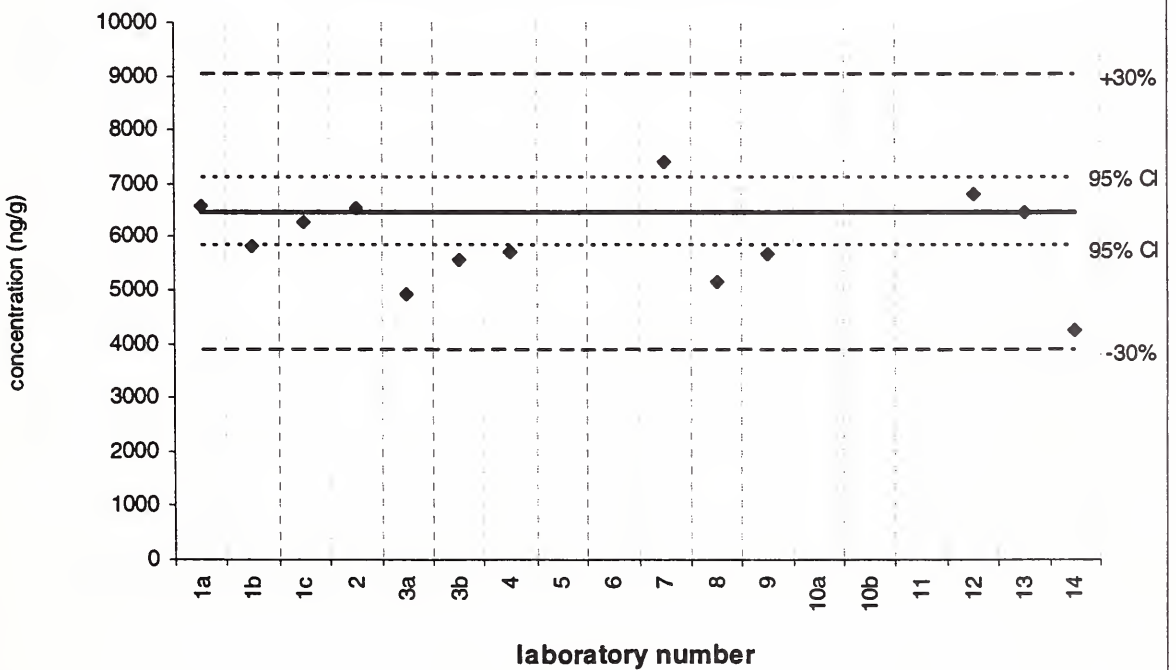


benzo[b]fluoranthene

SRM 1649a

Certified Value (solid line) = 6450 ± 640 ng/g

Reported Results: 13 Quantitative Results: 13

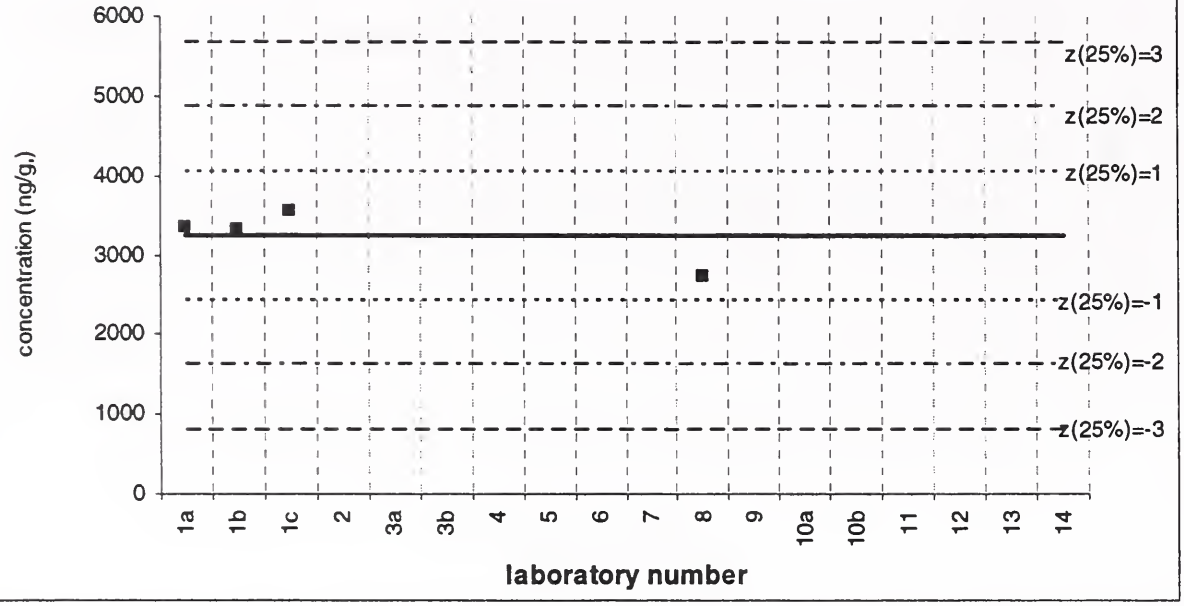


benzo[j]fluoranthene

SRM 1648

Assigned value (solid line) = 3237 ng/g s = 351 ng/g 95% CL = 559 ng/g

Reported Results: 4 Quantitative Results: 4

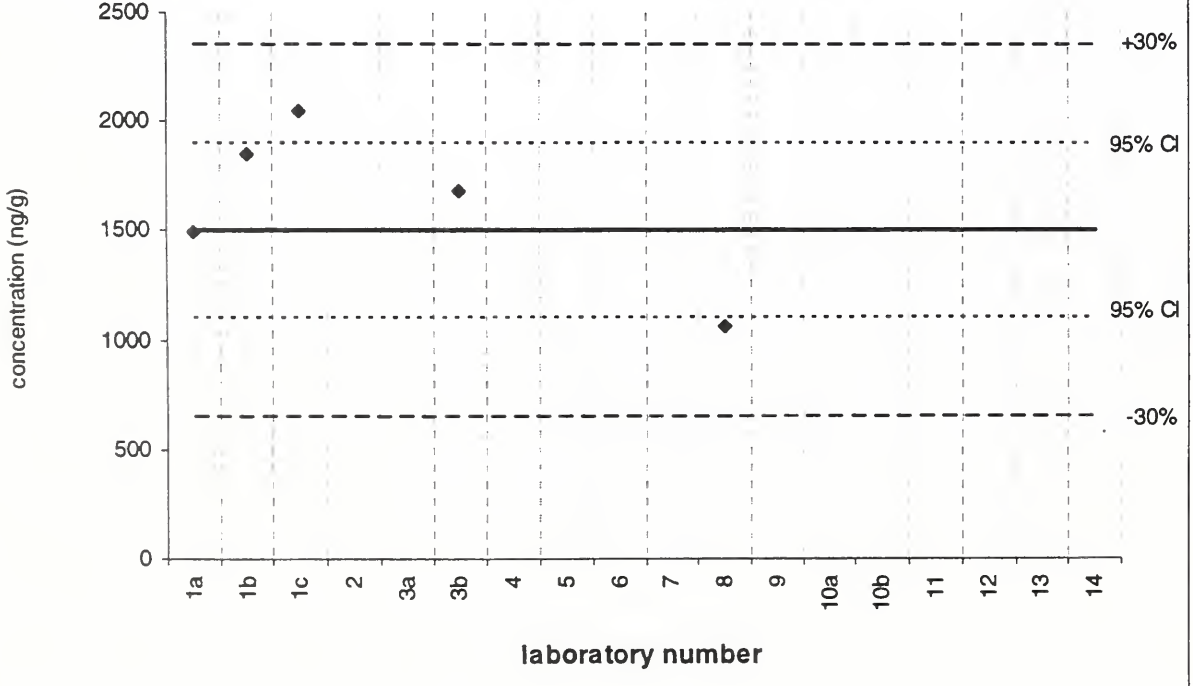


benzo[j]fluoranthene

SRM 1649a

Reference Value (solid line) = 1500 ± 400 ng/g

Reported Results: 5 Quantitative Results: 5

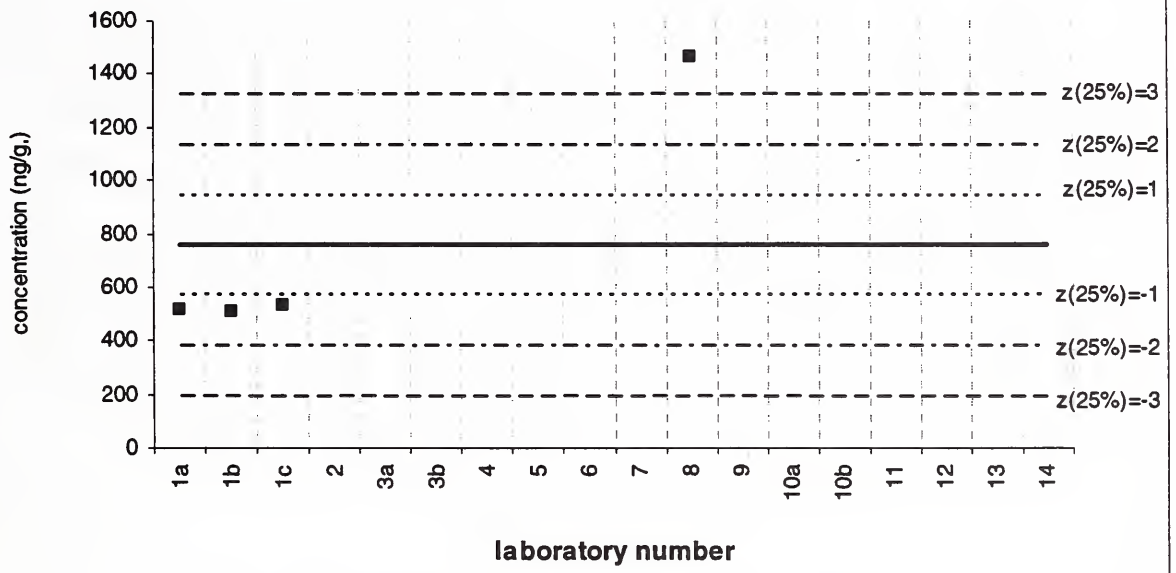


benzo[j]fluoranthene

Baltimore 2 PM

Assigned value (solid line) = 755 ng/g s = 473 ng/g 95% CL = 752 ng/g

Reported Results: 5 Quantitative Results: 4

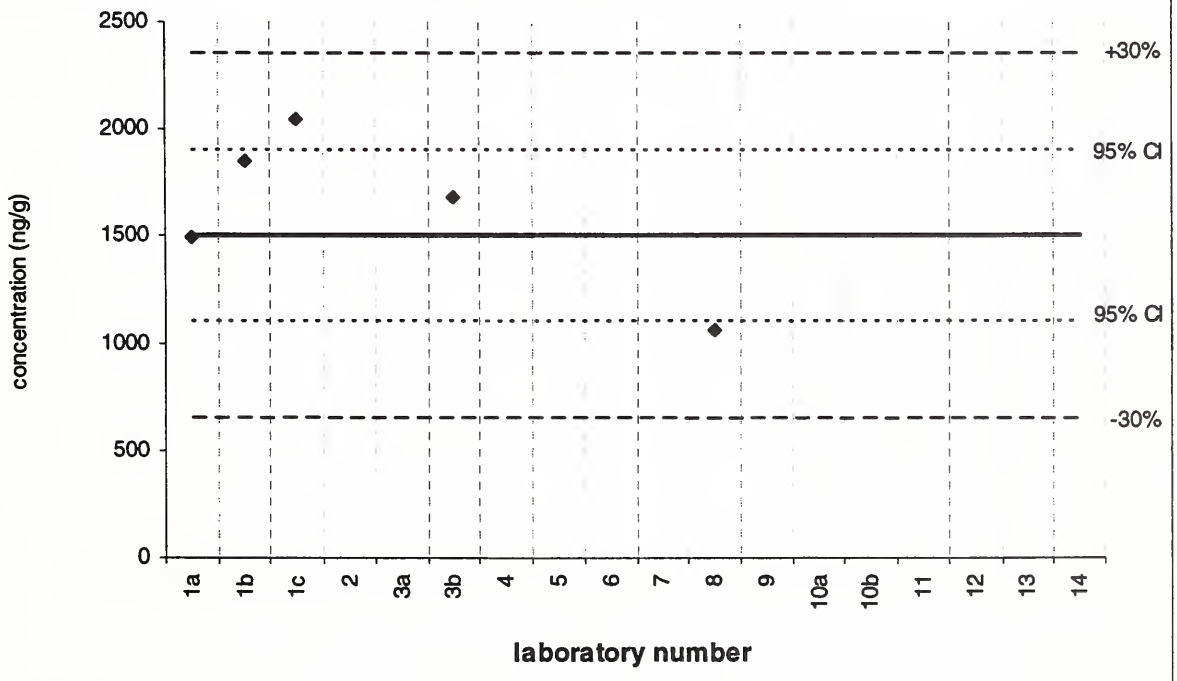


benzo[j]fluoranthene

SRM 1649a

Reference Value (solid line) = 1500 ± 400 ng/g

Reported Results: 5 Quantitative Results: 5

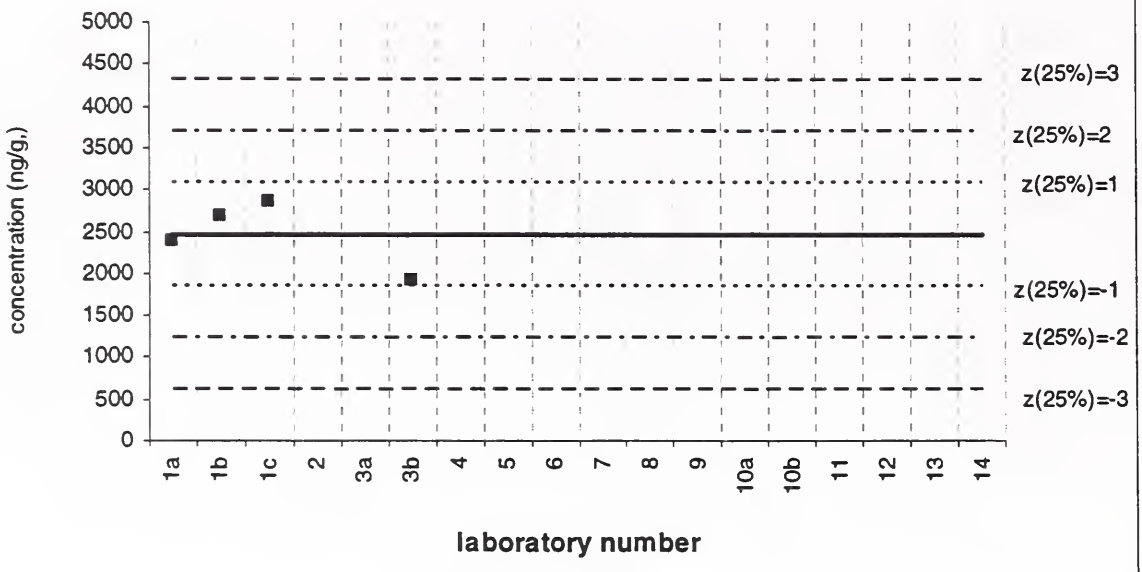


benzo[j]fluoranthene

Filter samples

Assigned value (solid line) = 2461 ng/g s = 416 ng/g 95% CL = 663 ng/g

Reported Results: 6 Quantitative Results: 4

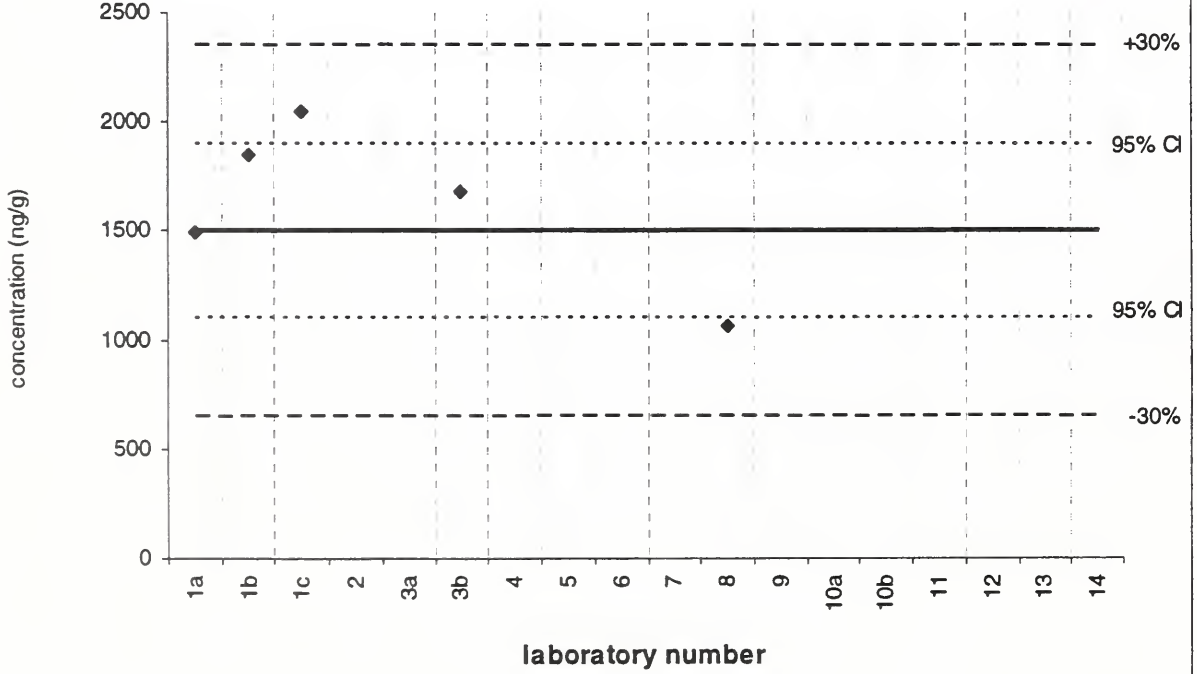


benzo[j]fluoranthene

SRM 1649a

Reference Value (solid line) = 1500 ± 400 ng/g

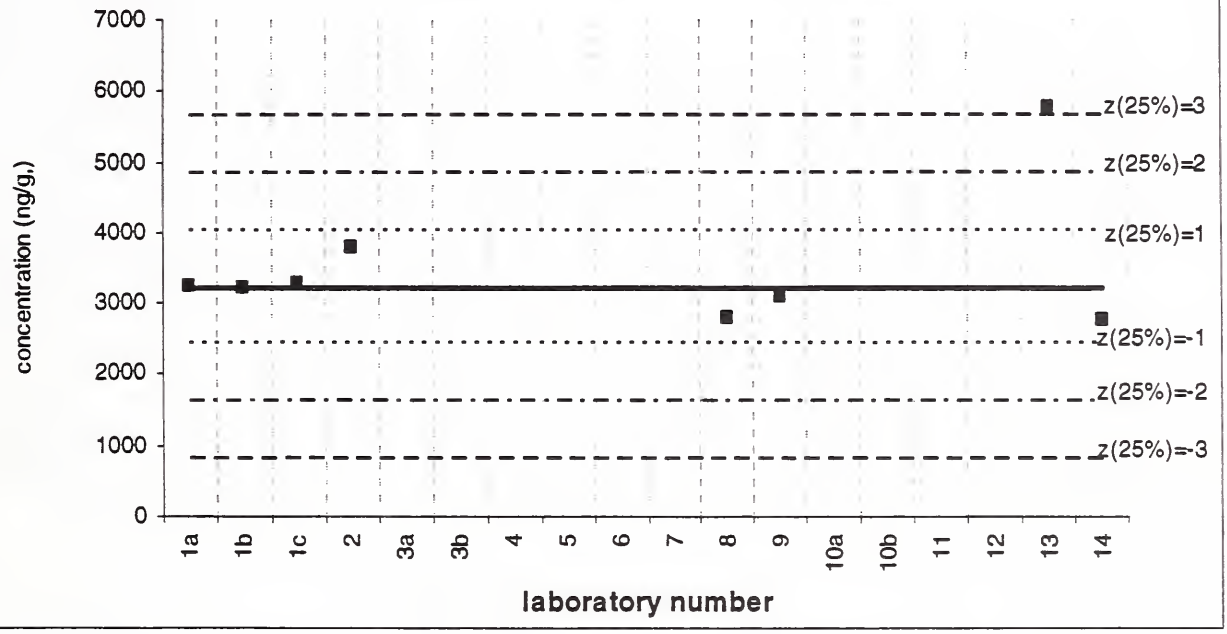
Reported Results: 5 Quantitative Results: 5



benzo[k]fluoranthene SRM 1648

Assigned value (solid line) = 3228 ng/g s = 336 ng/g 95% CL = 352 ng/g

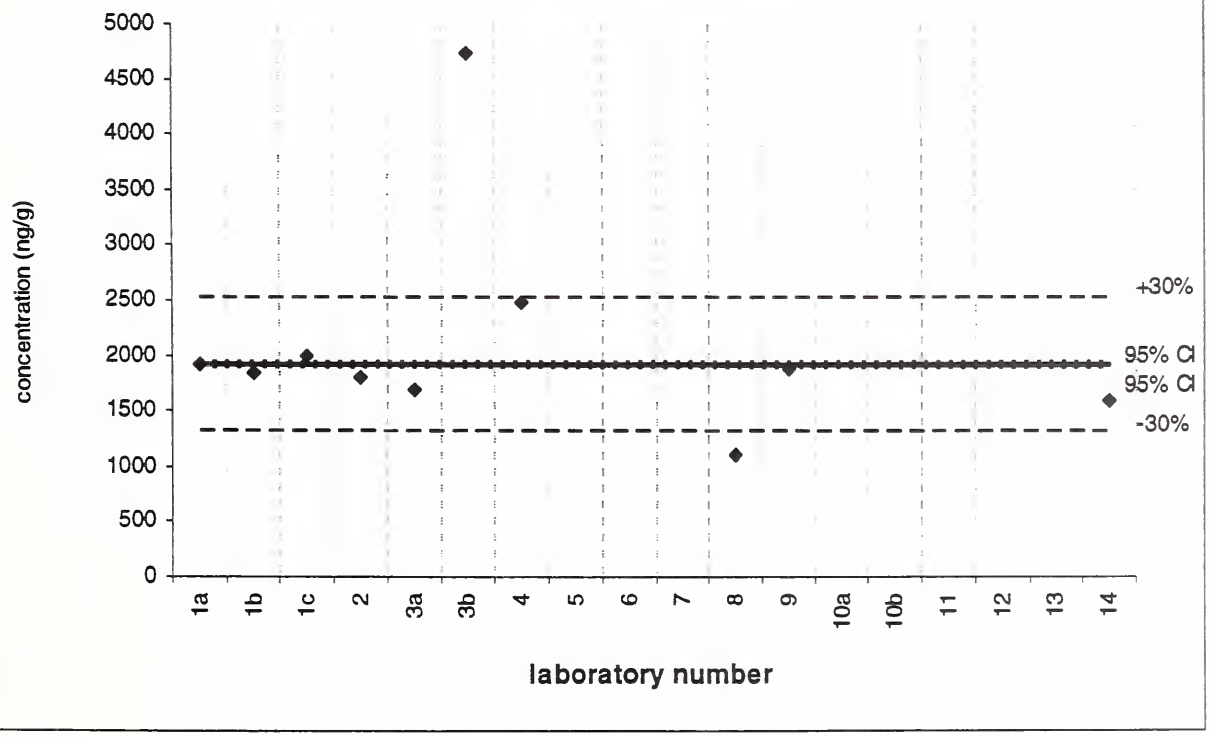
Reported Results: 8 Quantitative Results: 8



benzo[k]fluoranthene SRM 1649a

Certified Value (solid line) = 1913 ± 31 ng/g

Reported Results: 10 Quantitative Results: 10

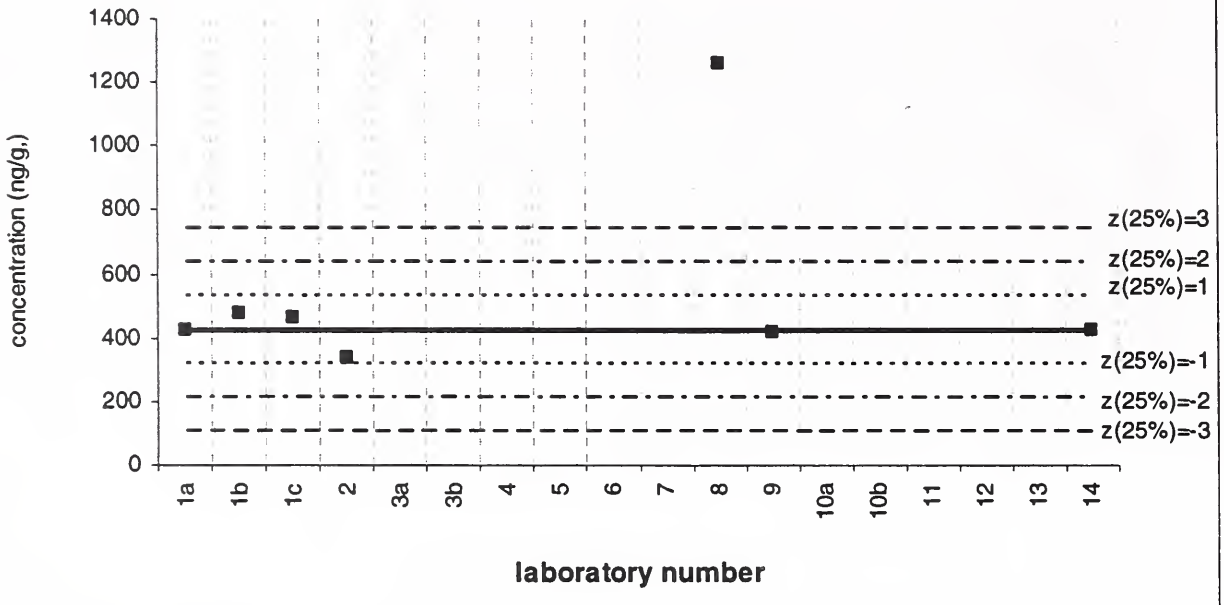


benzo[k]fluoranthene

Baltimore 2 PM

Assigned value (solid line) = 424 ng/g s = 48 ng/g 95% CL = 51 ng/g

Reported Results: 8 Quantitative Results: 7

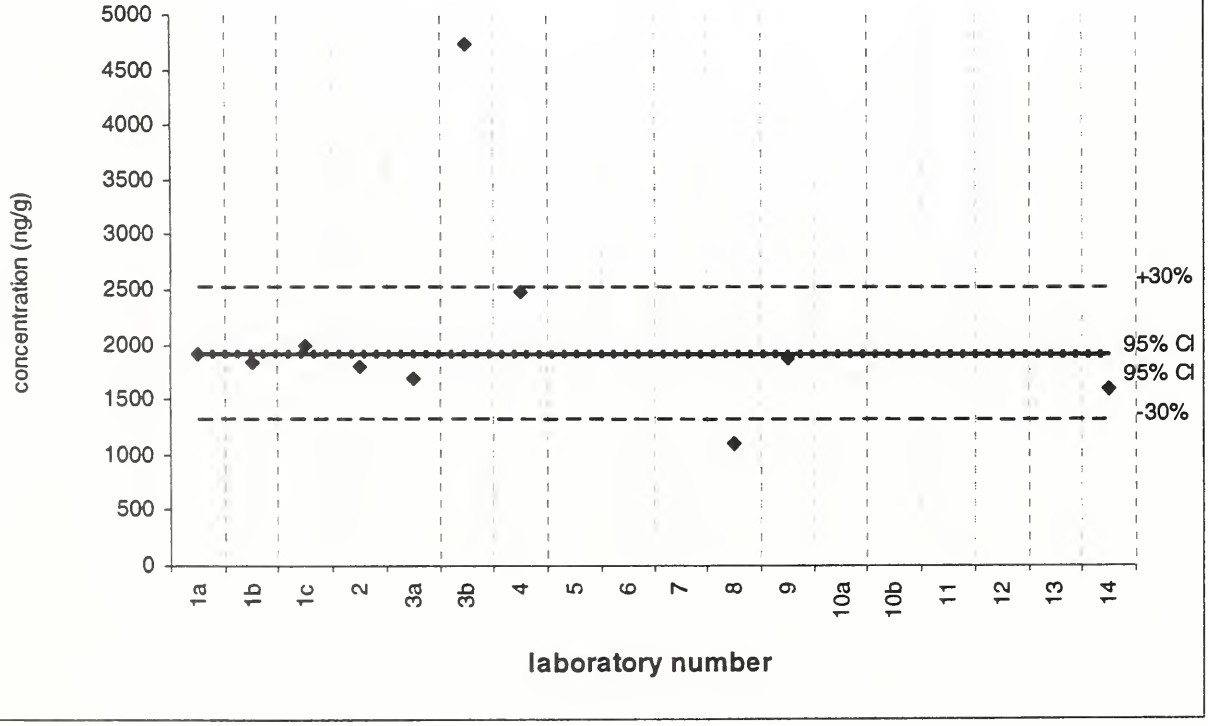


benzo[k]fluoranthene

SRM 1649a

Certified Value (solid line) = 1913 ± 31 ng/g

Reported Results: 10 Quantitative Results: 10

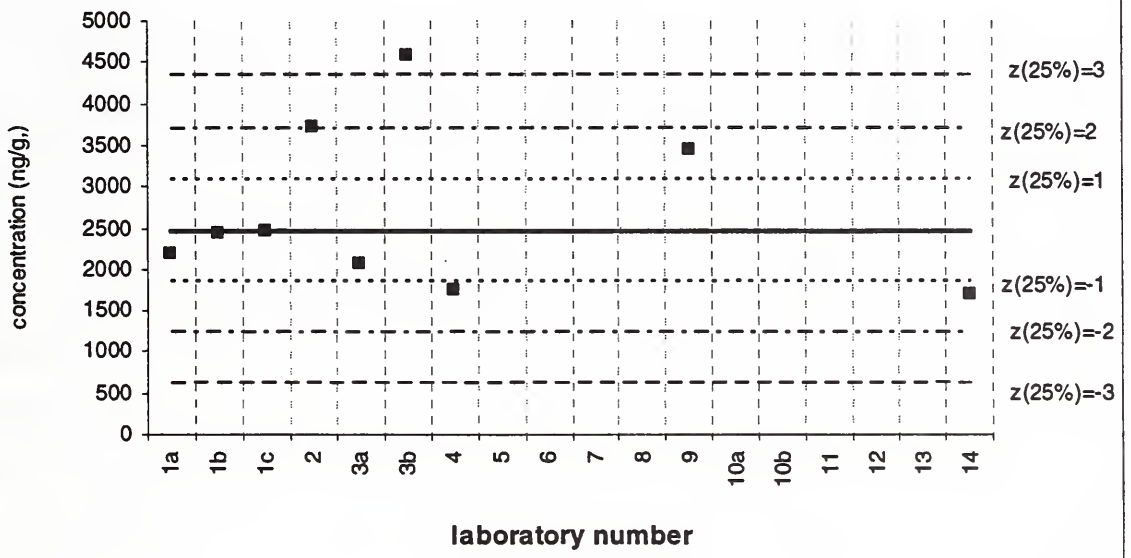


benzo[k]fluoranthene

Filter samples

Assigned value (solid line) = 2470 ng/g s = 742 ng/g 95% CL = 621 ng/g

Reported Results: 11 Quantitative Results: 9

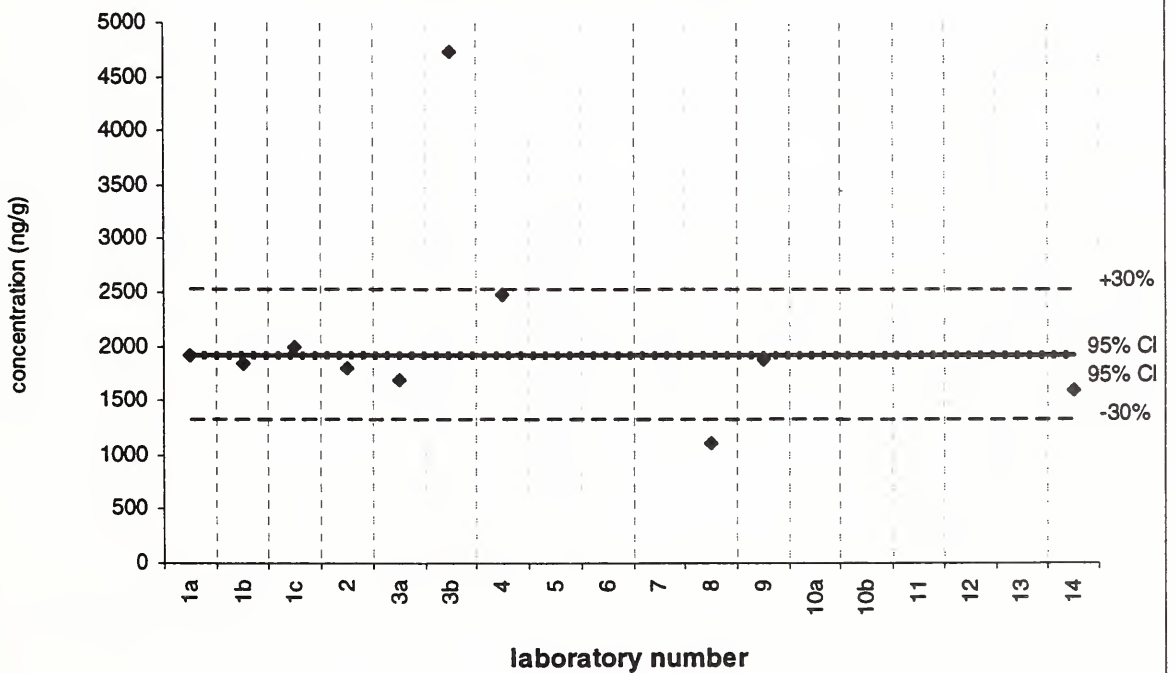


benzo[k]fluoranthene

SRM 1649a

Certified Value (solid line) = 1913 ± 31 ng/g

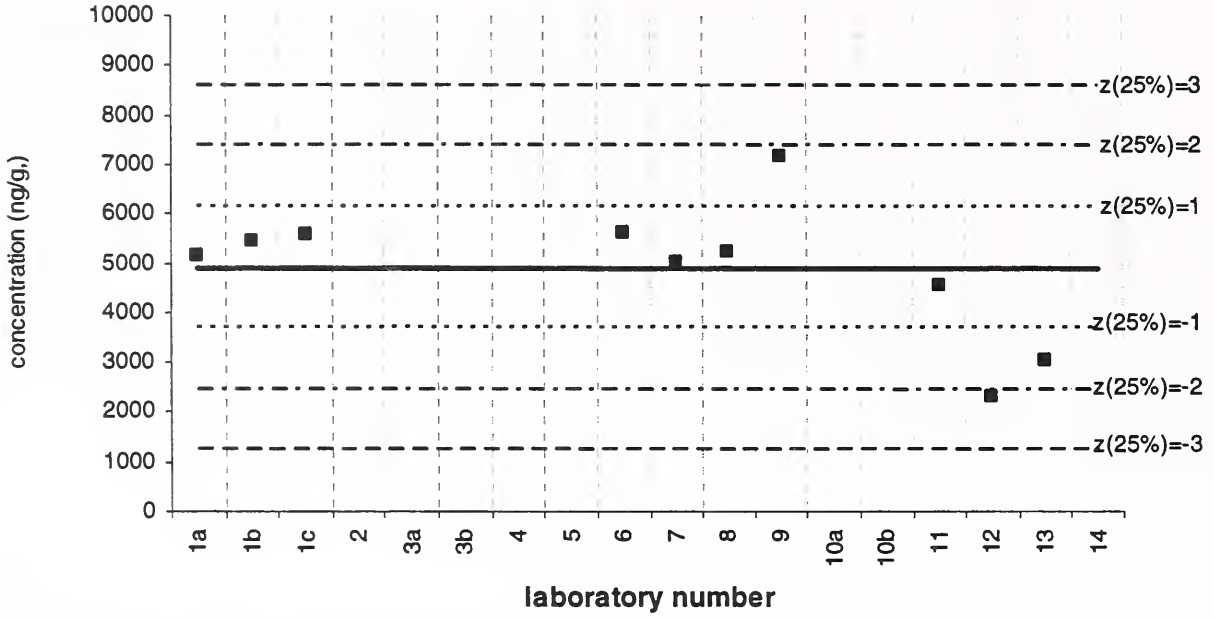
Reported Results: 10 Quantitative Results: 10



benzo[e]pyrene

SRM 1648

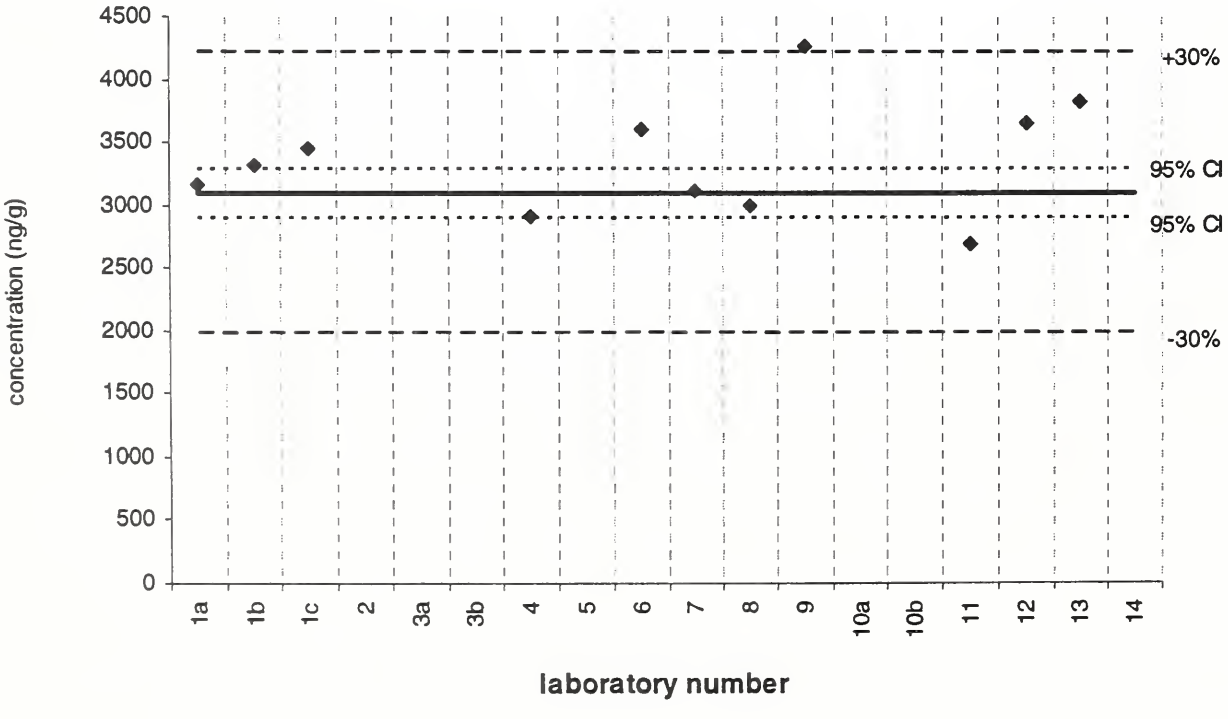
Assigned value (solid line) = 4913 ng/g s = 1368 ng/g 95% CL = 979 ng/g
Reported Results: 10 Quantitative Results: 10



benzo[e]pyrene

SRM 1649a

Certified Value (solid line) = 3090 ± 190 ng/g
Reported Results: 11 Quantitative Results: 11

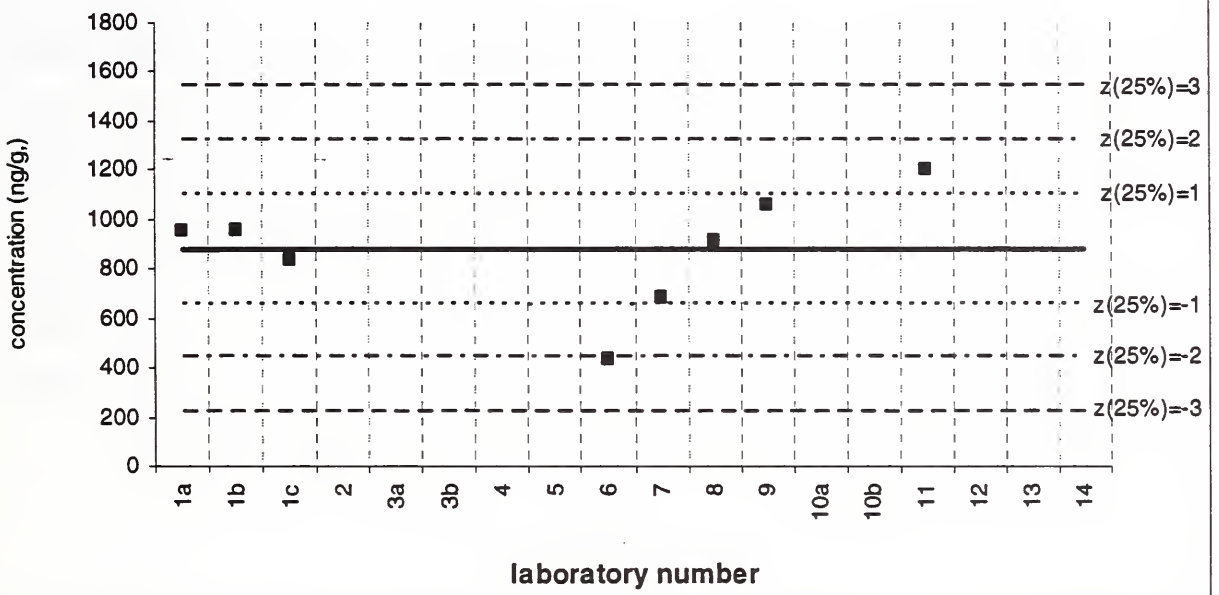


benzo[e]pyrene

Baltimore 2 PM

Assigned value (solid line) = 881 ng/g s = 236 ng/g 95% CL = 197 ng/g

Reported Results: 9 Quantitative Results: 8

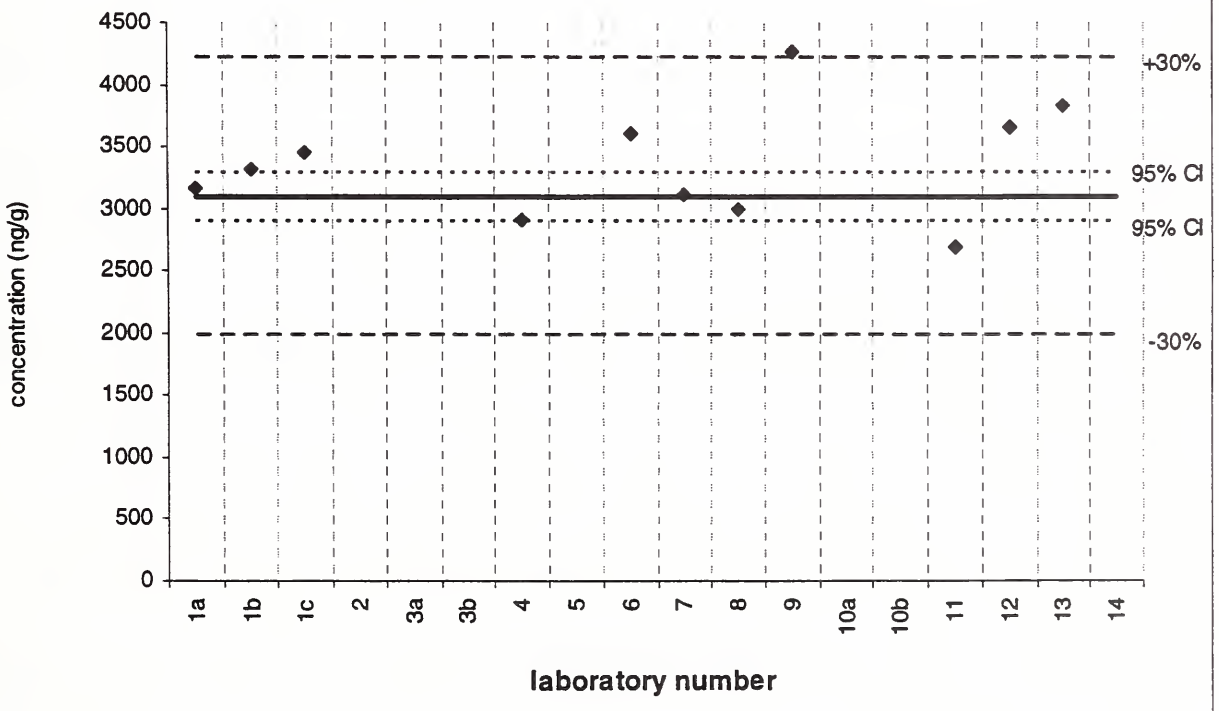


benzo[e]pyrene

SRM 1649a

Certified Value (solid line) = 3090 ± 190 ng/g

Reported Results: 11 Quantitative Results: 11

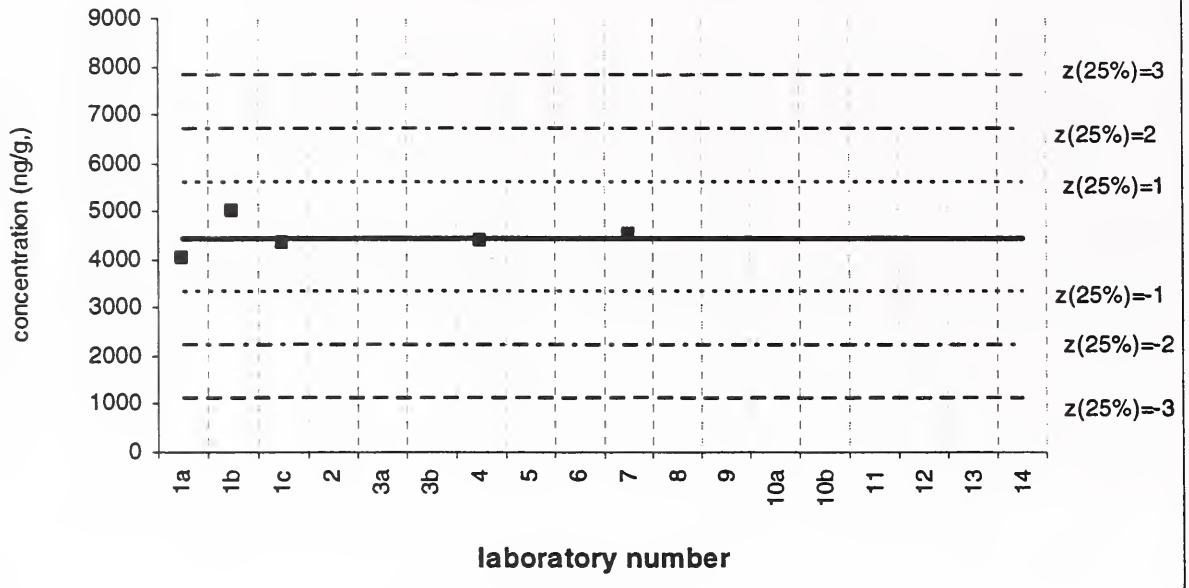


benzo[e]pyrene

Filter samples

Assigned value (solid line) = 4452 ng/g s = 365 ng/g 95% CL = 453 ng/g

Reported Results: 9 Quantitative Results: 7



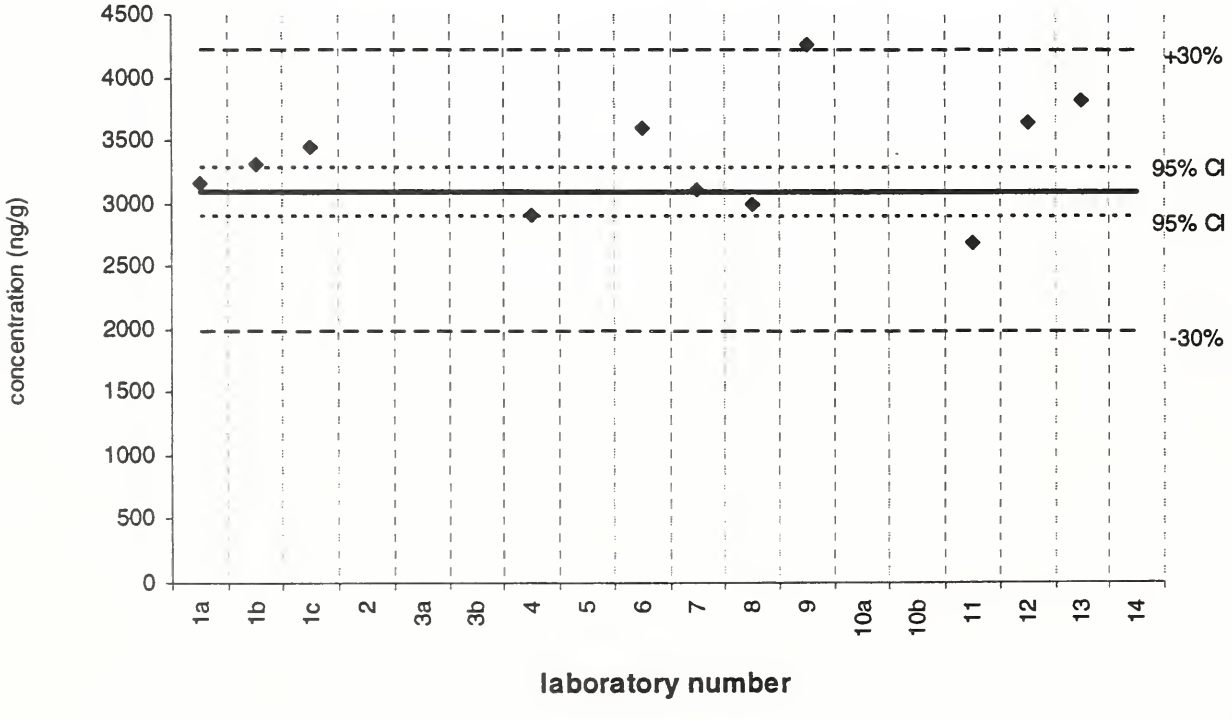
Lab 9 = 39970 ng/g; lab 11 = 18668 ng/g

benzo[e]pyrene

SRM 1649a

Certified Value (solid line) = 3090 ± 190 ng/g

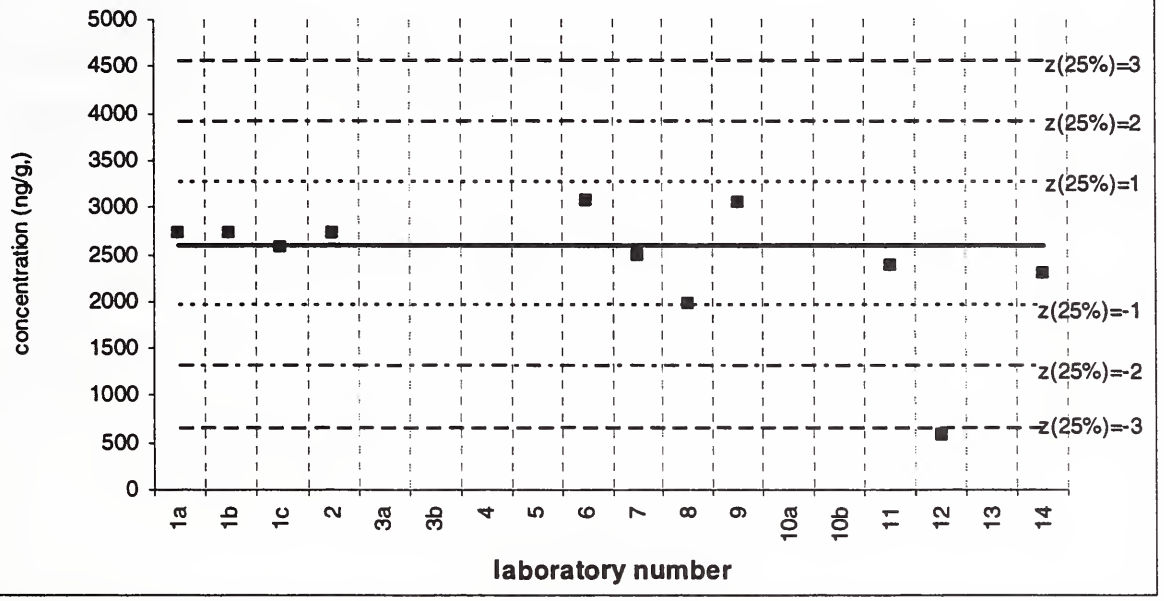
Reported Results: 11 Quantitative Results: 11



benzo[a]pyrene

SRM 1648

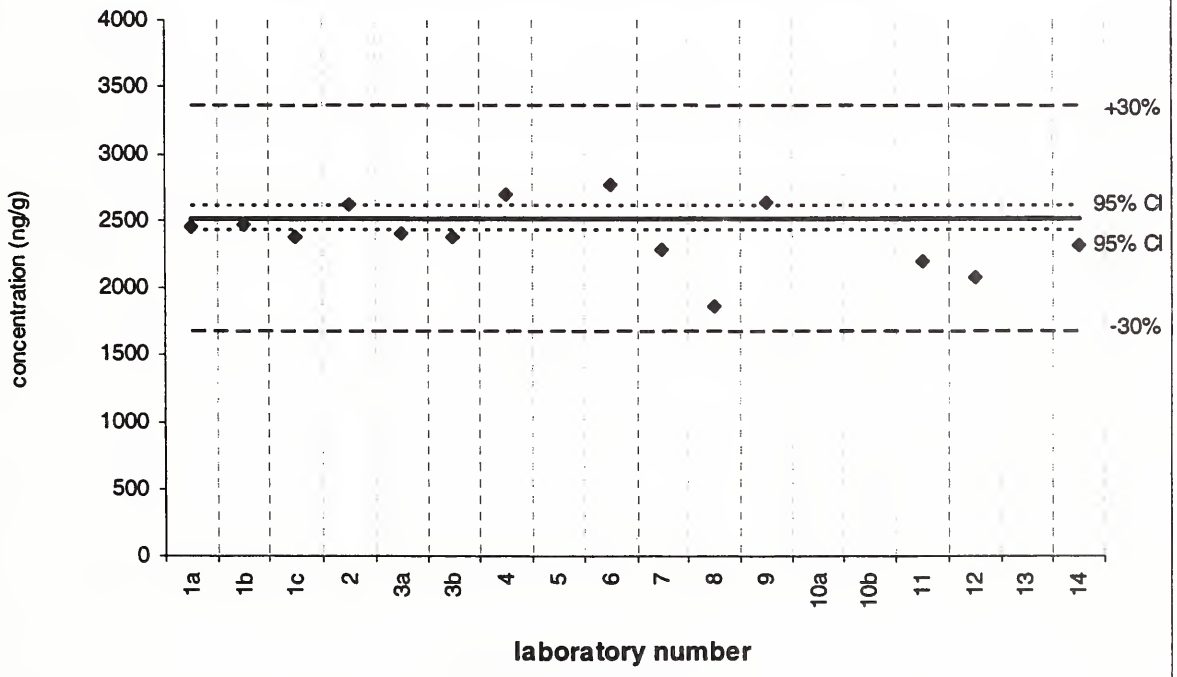
Assigned value (solid line) = 2601 ng/g s = 335 ng/g 95% CL = 239 ng/g
Reported Results: 11 Quantitative Results: 11

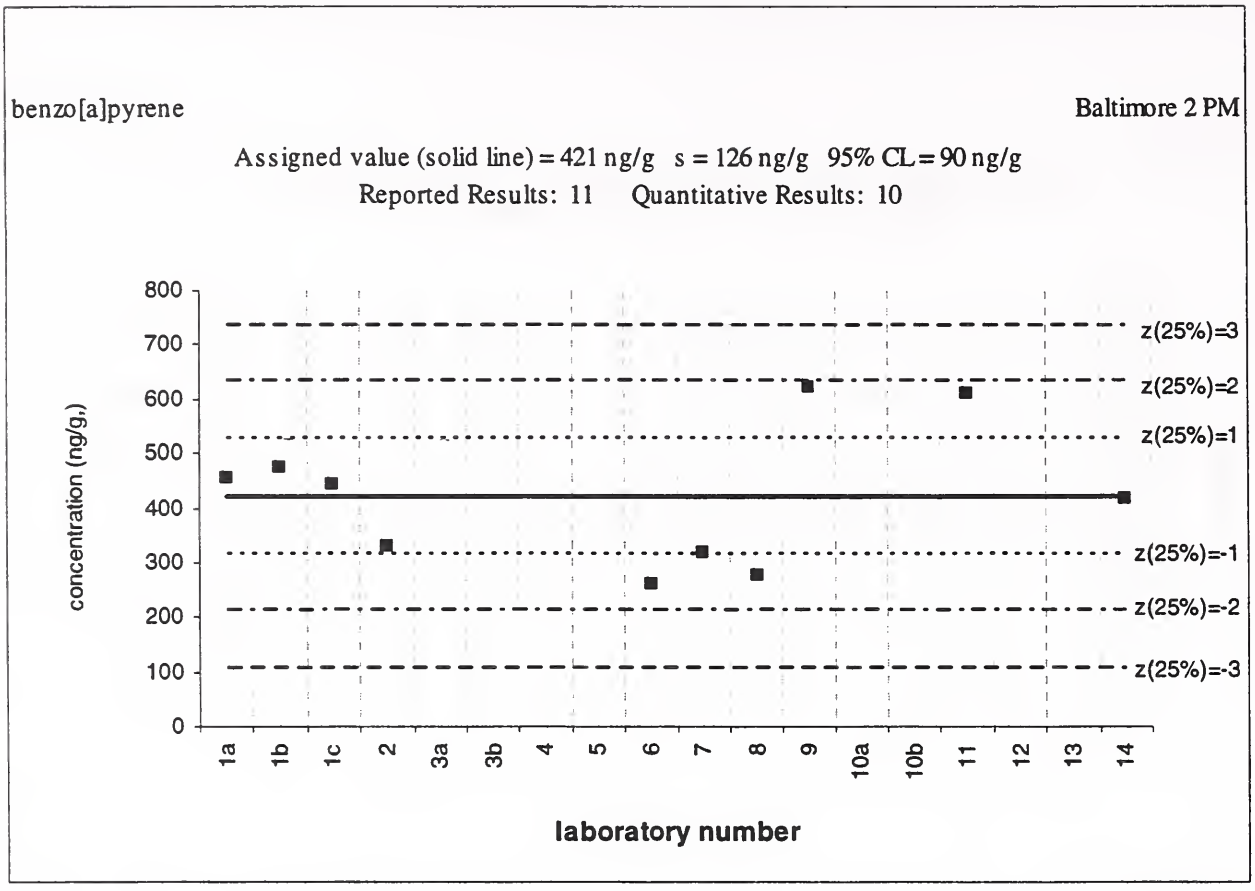


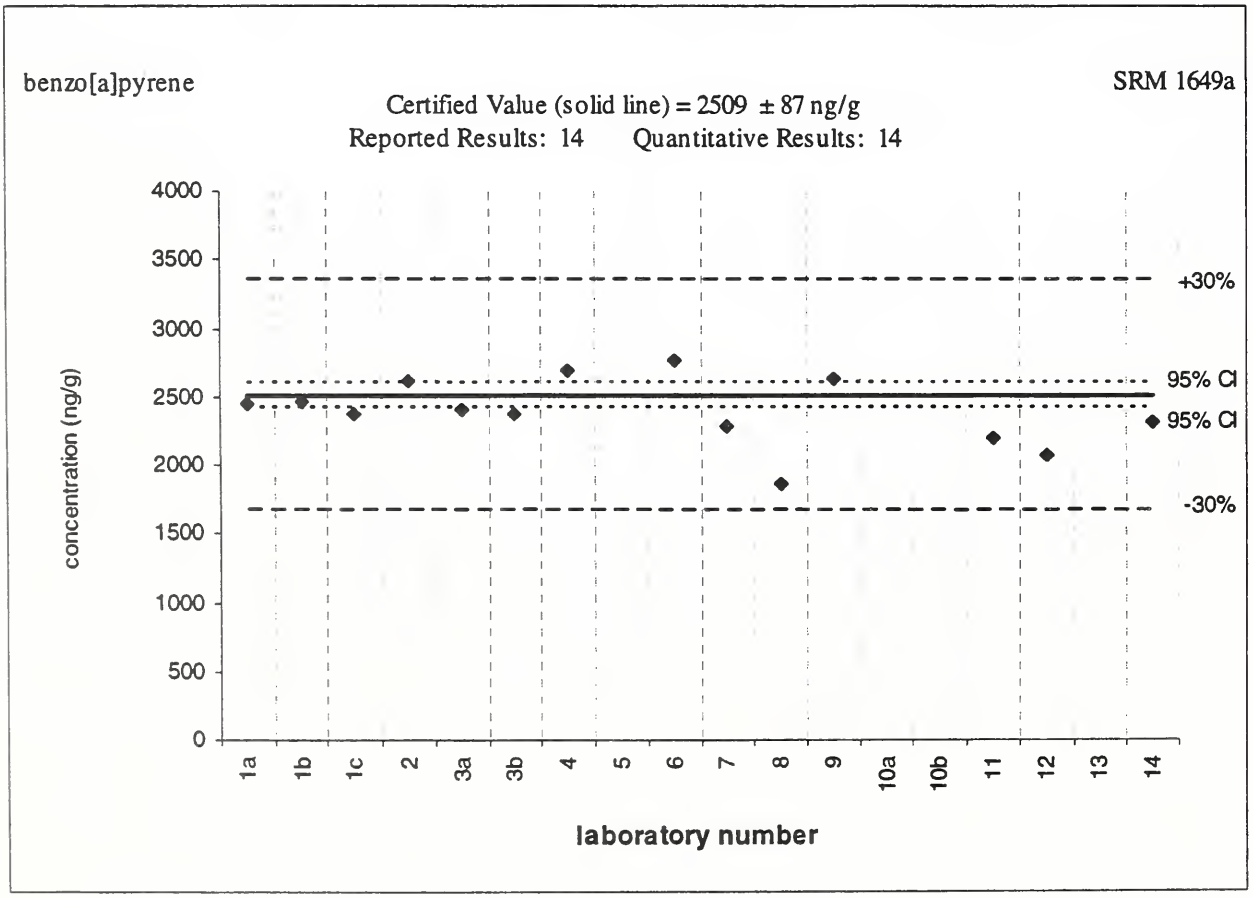
benzo[a]pyrene

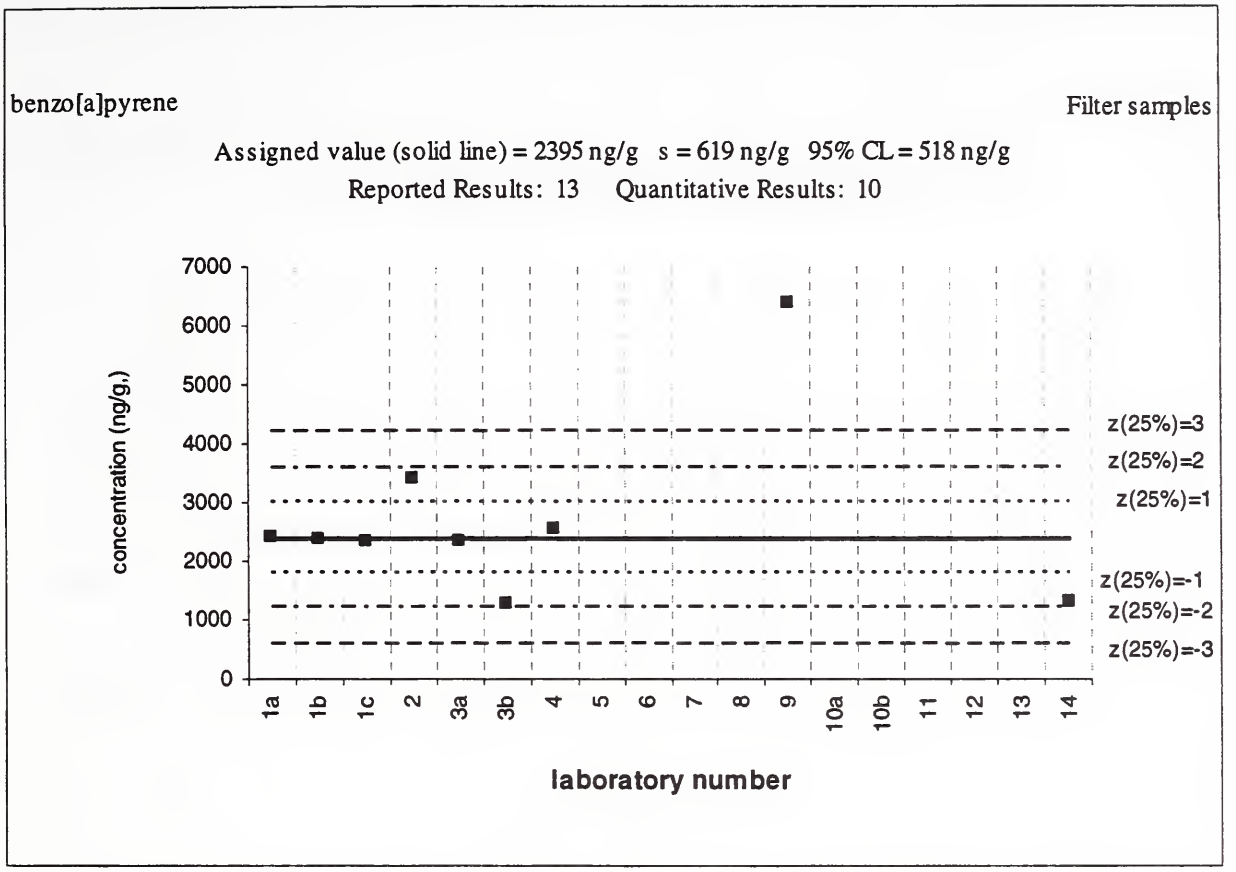
SRM 1649a

Certified Value (solid line) = 2509 ± 87 ng/g
Reported Results: 14 Quantitative Results: 14

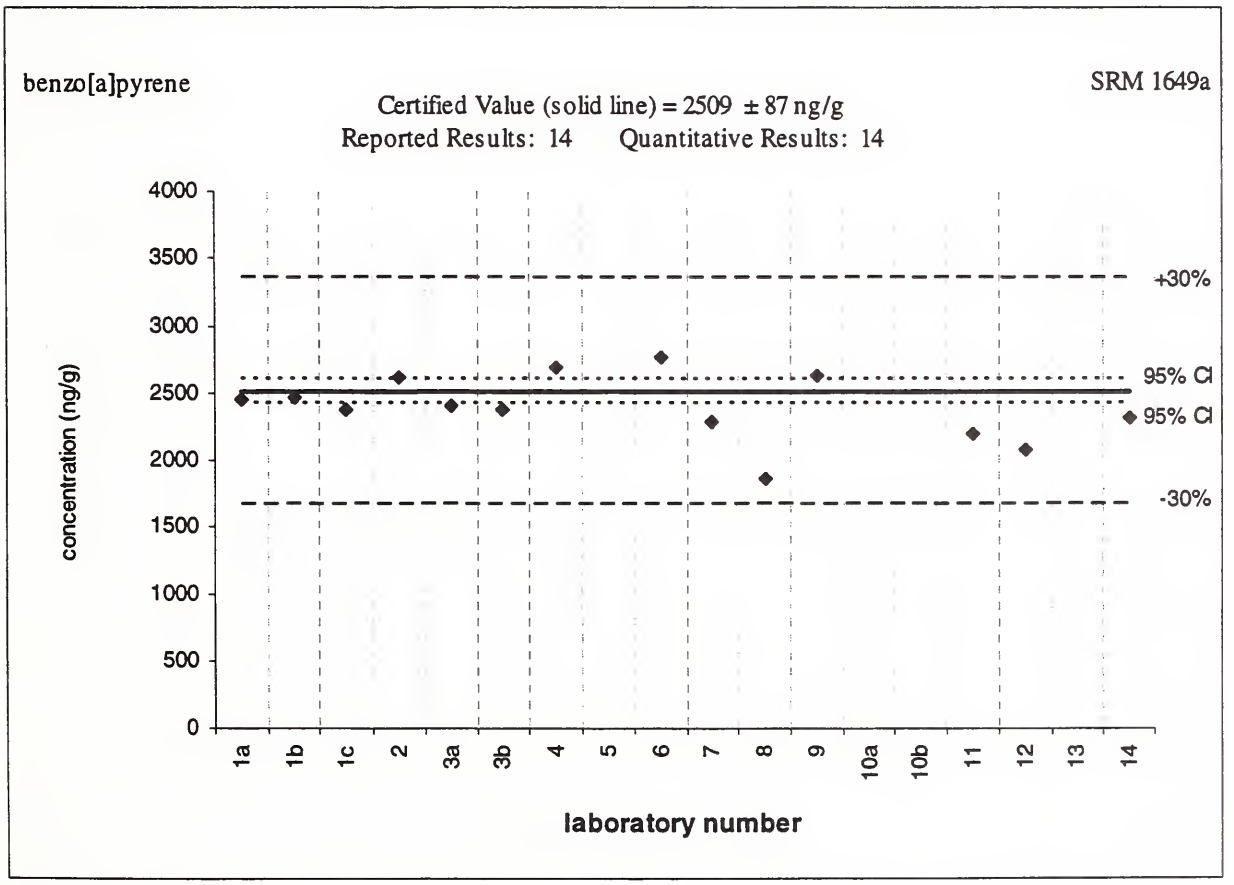



benzo[a]pyrene
Baltimore 2 PM
Assigned value (solid line) = 421 ng/g s = 126 ng/g 95% CL = 90 ng/g
Reported Results: 11 Quantitative Results: 10
concentration (ng/g,)
800
700
600
500
400
300
200
100
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number


benzo[a]pyrene
SRM 1649a
Certified Value (solid line) = 2509 ± 87 ng/g
Reported Results: 14 Quantitative Results: 14
concentration (ng/g)
4000
3500
3000
2500
2000
1500
1000
500
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number



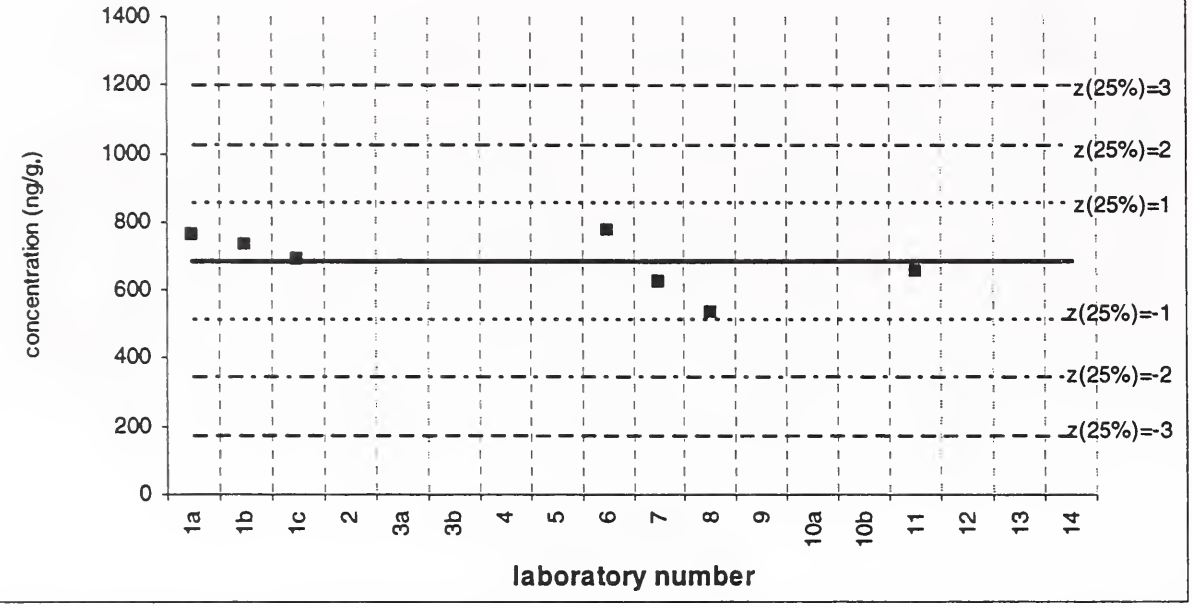
lab 11 = 18014 ng/g



perylene

SRM 1648

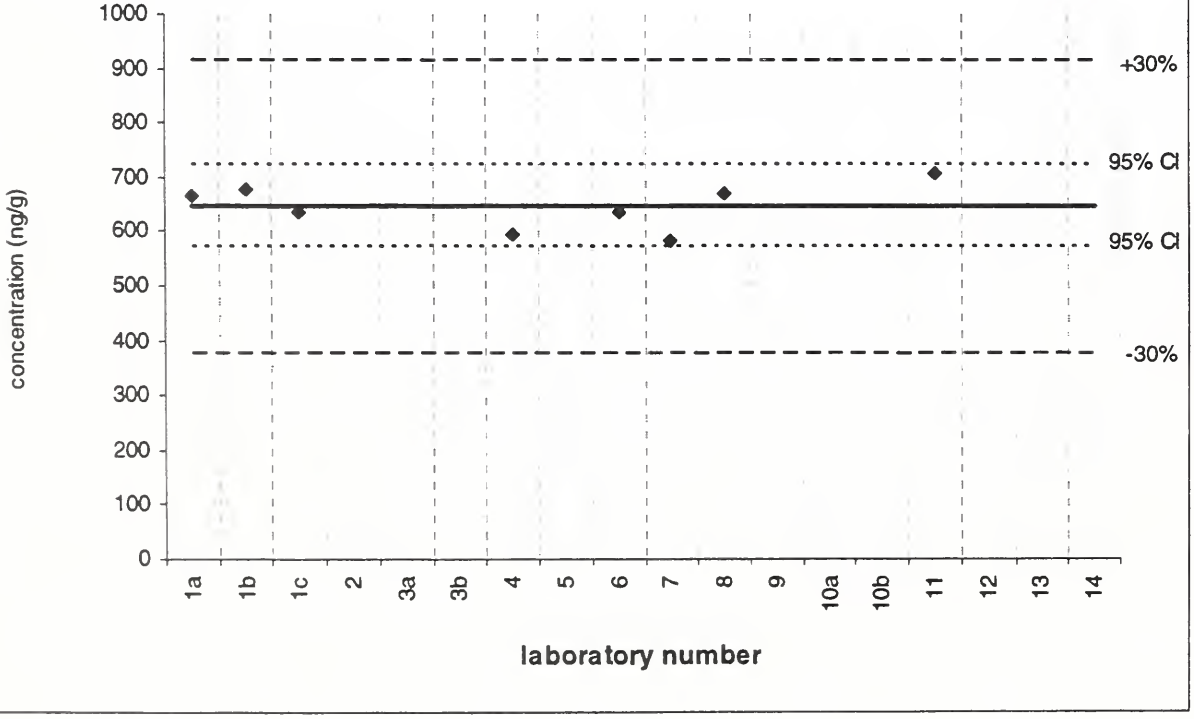
Assigned value (solid line) = 682 ng/g s = 86 ng/g 95% CL = 80 ng/g
Reported Results: 8 Quantitative Results: 7



perylene

SRM 1649a

Certified Value (solid line) = 646 ± 75 ng/g
Reported Results: 9 Quantitative Results: 8

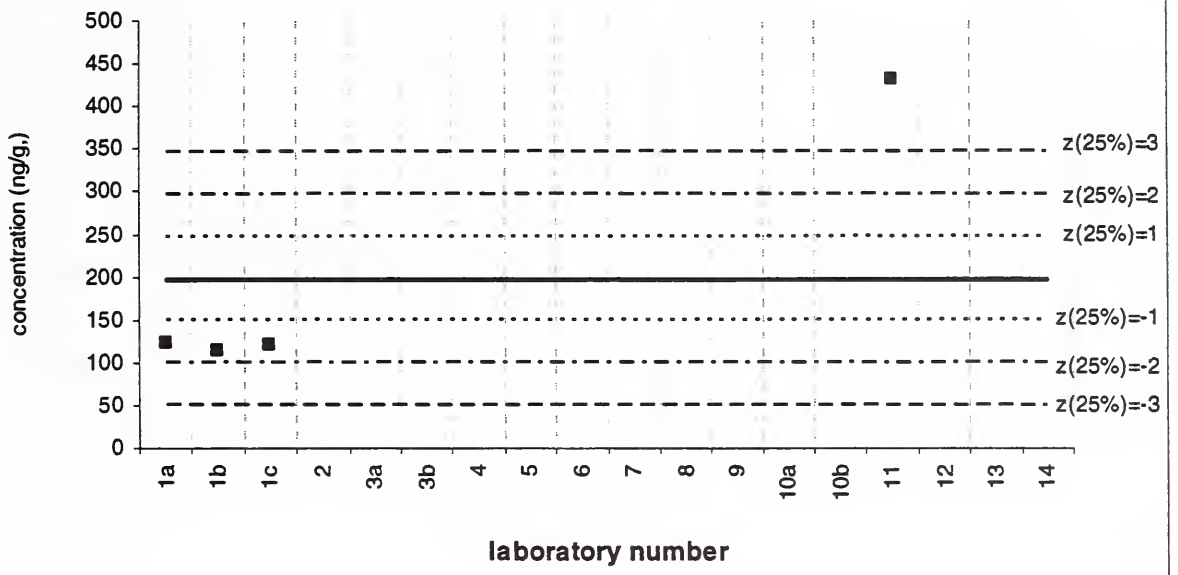


perylene

Baltimore 2 PM

Assigned value (solid line) = 198 ng/g s = 156 ng/g 95% CL = 248 ng/g

Reported Results: 8 Quantitative Results: 4

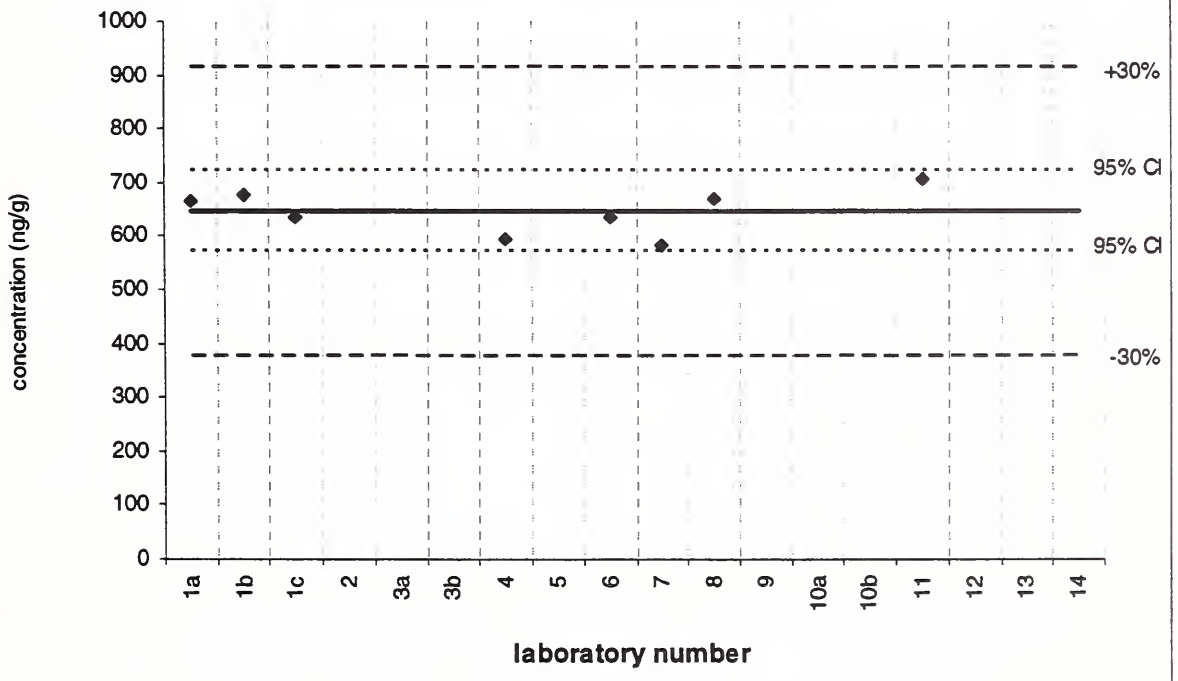


perylene

SRM 1649a

Certified Value (solid line) = 646 ± 75 ng/g

Reported Results: 9 Quantitative Results: 8

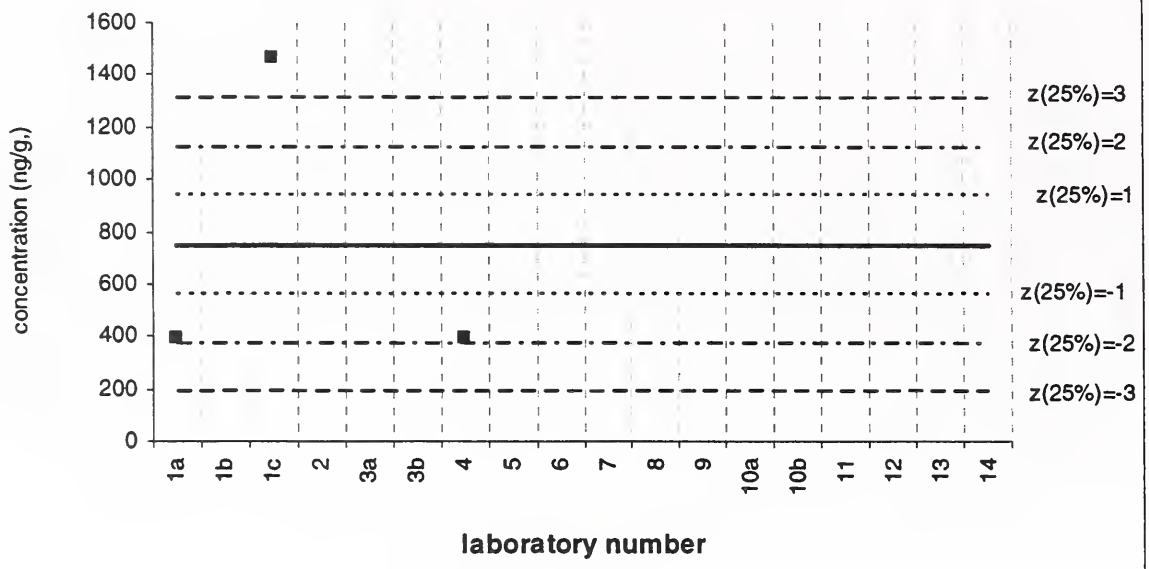


perylene

Filter samples

Assigned value (solid line) = 748 ng/g s = 619 ng/g 95% CL = 1537 ng/g

Reported Results: 8 Quantitative Results: 4



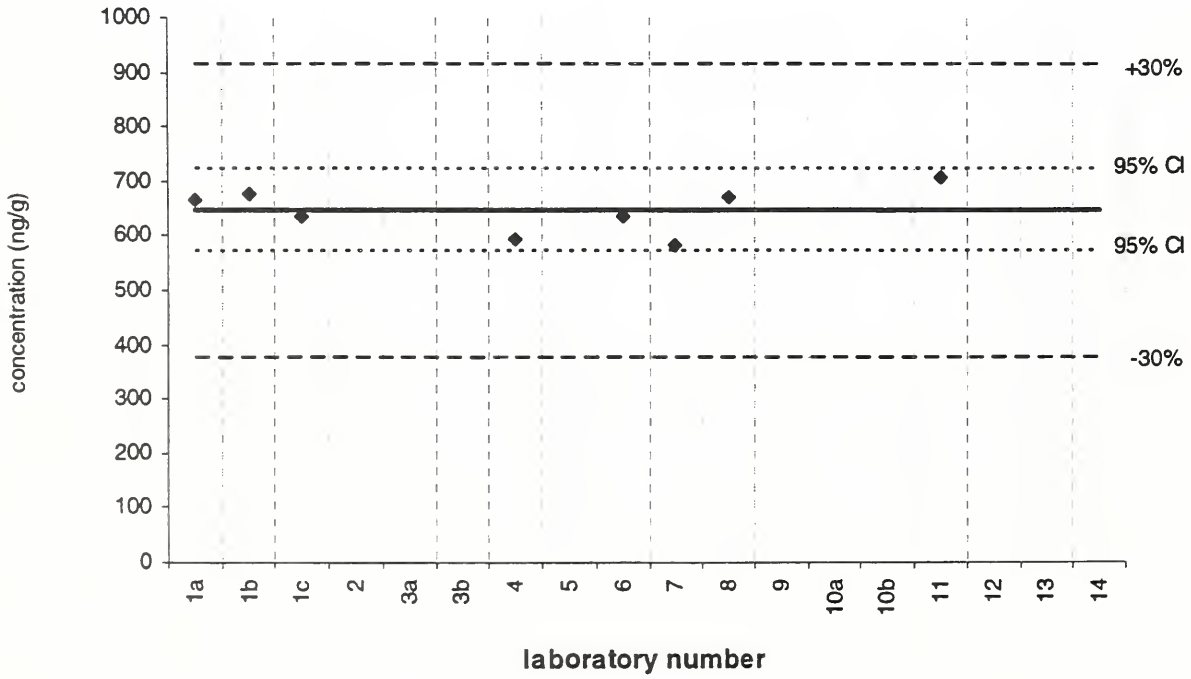
lab 11 = 14926 ng/g

perylene

SRM 1649a

Certified Value (solid line) = 646 ± 75 ng/g

Reported Results: 9 Quantitative Results: 8

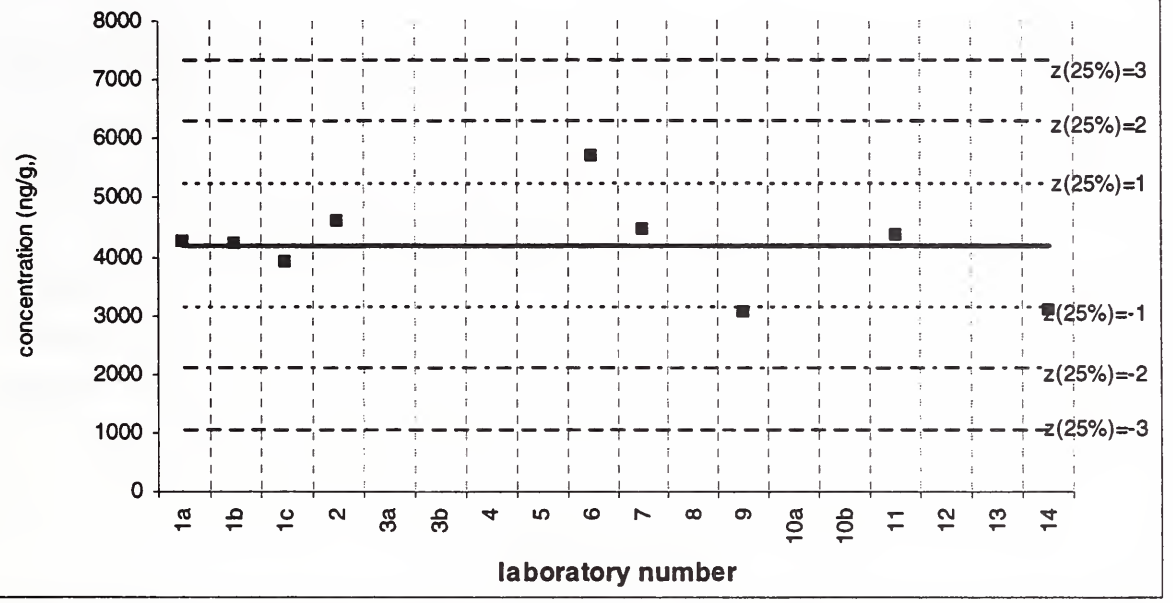


indeno[1,2,3-cd]pyrene

SRM 1648

Assigned value (solid line) = 4187 ng/g s = 801 ng/g 95% CL = 616 ng/g

Reported Results: 10 Quantitative Results: 9

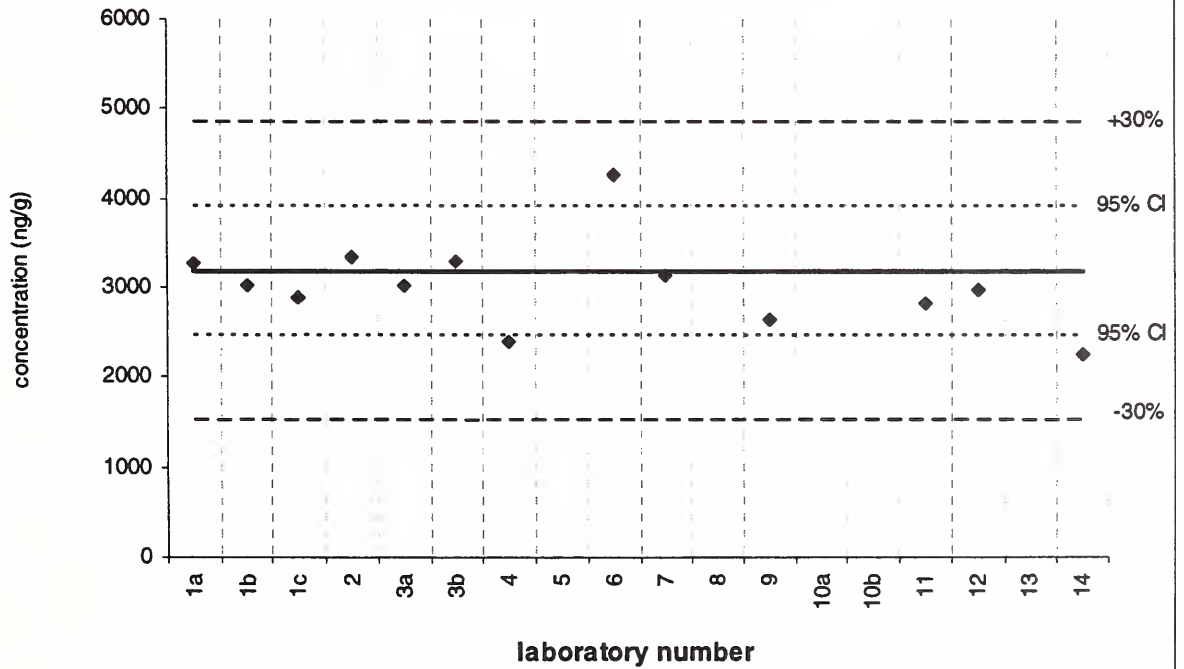


indeno[1,2,3-cd]pyrene

SRM 1649a

Certified Value (solid line) = 3180 ± 720 ng/g

Reported Results: 13 Quantitative Results: 13

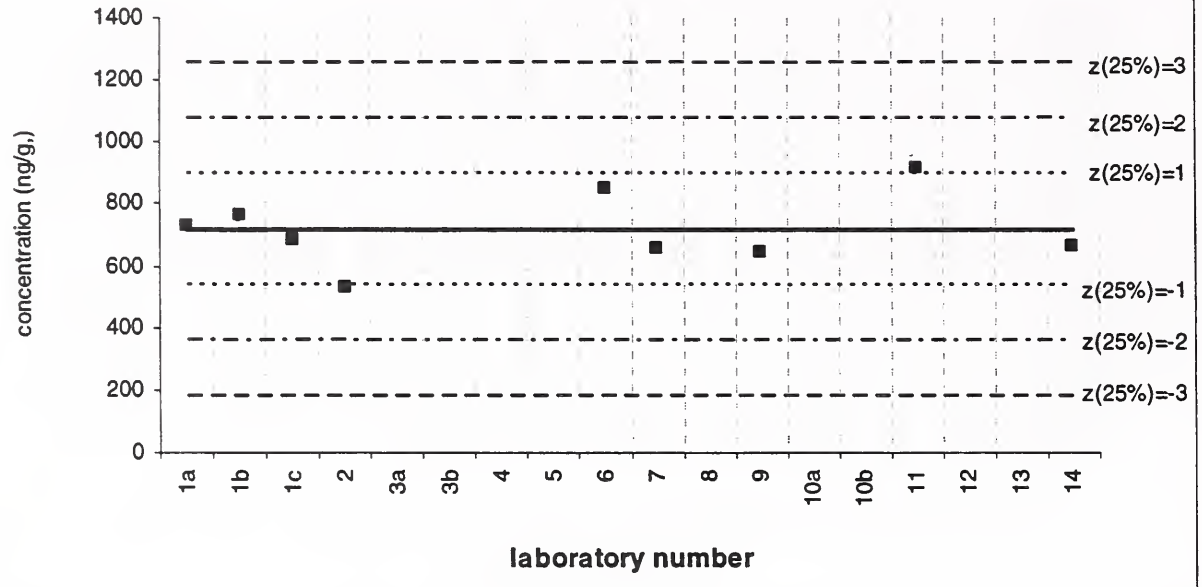


indeno[1,2,3-cd]pyrene

Baltimore 2 PM

Assigned value (solid line) = 716 ng/g s = 115 ng/g 95% CL = 89 ng/g

Reported Results: 10 Quantitative Results: 9

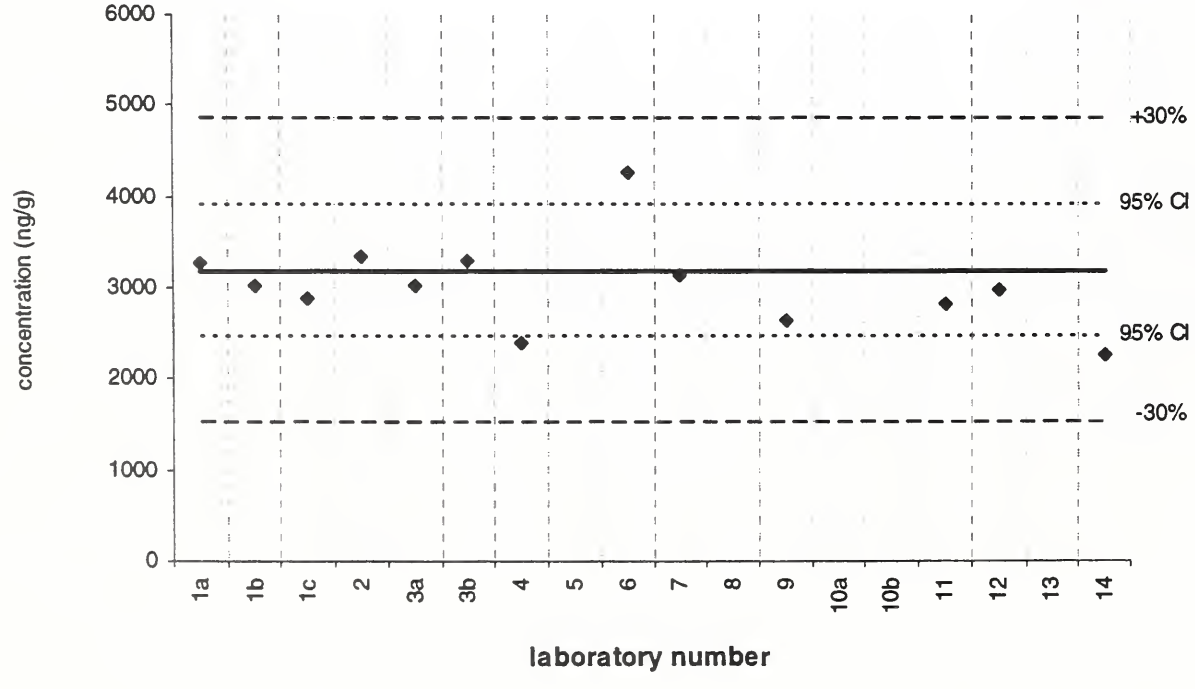


indeno[1,2,3-cd]pyrene

SRM 1649a

Certified Value (solid line) = 3180 ± 720 ng/g

Reported Results: 13 Quantitative Results: 13



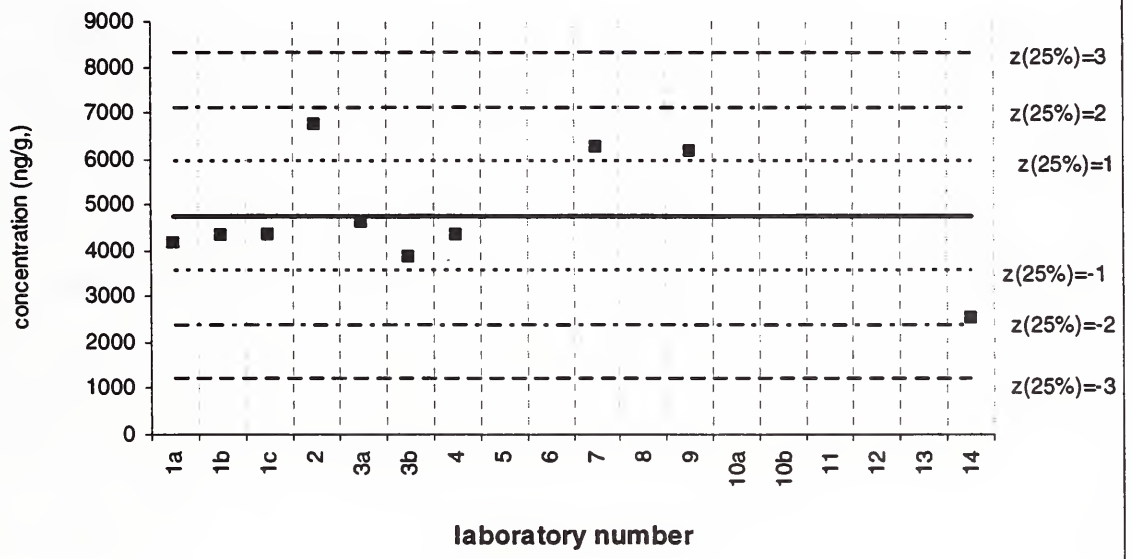
indeno[1,2,3-cd]pyrene

Filter samples

Assigned value (solid line) = 4737 ng/g s = 1279 ng/g 95% CL = 915 ng/g

Reported Results: 12 Quantitative Results: 11

lab 11 = 21364 ng/g

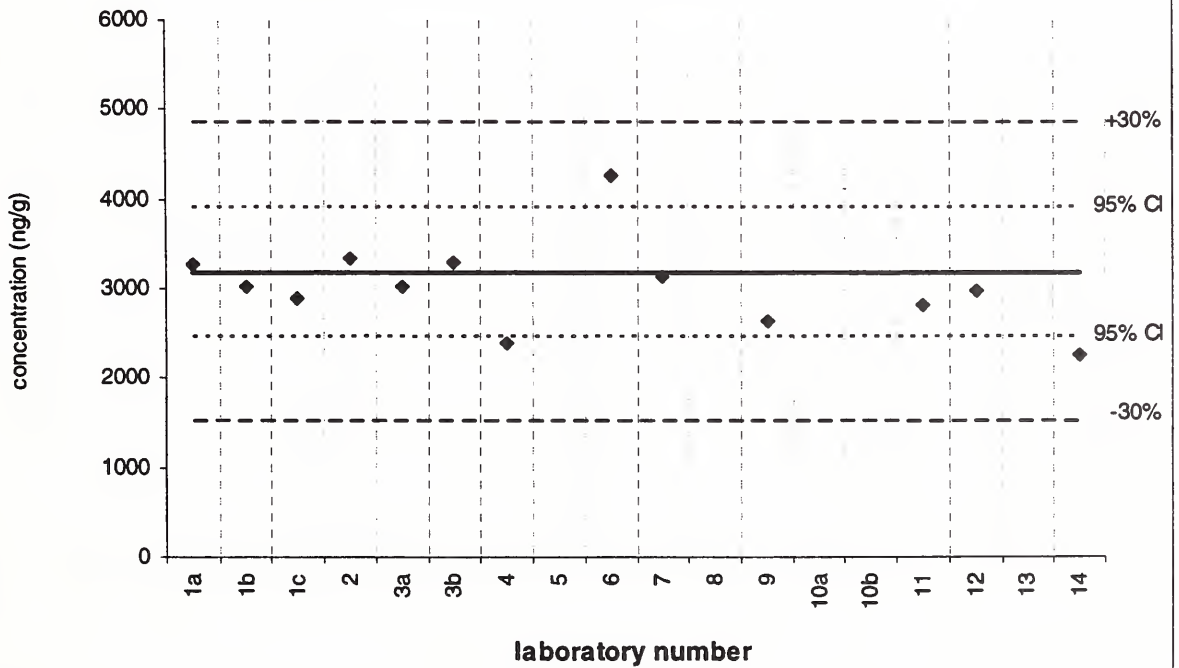


indeno[1,2,3-cd]pyrene

SRM 1649a

Certified Value (solid line) = 3180 ± 720 ng/g

Reported Results: 13 Quantitative Results: 13

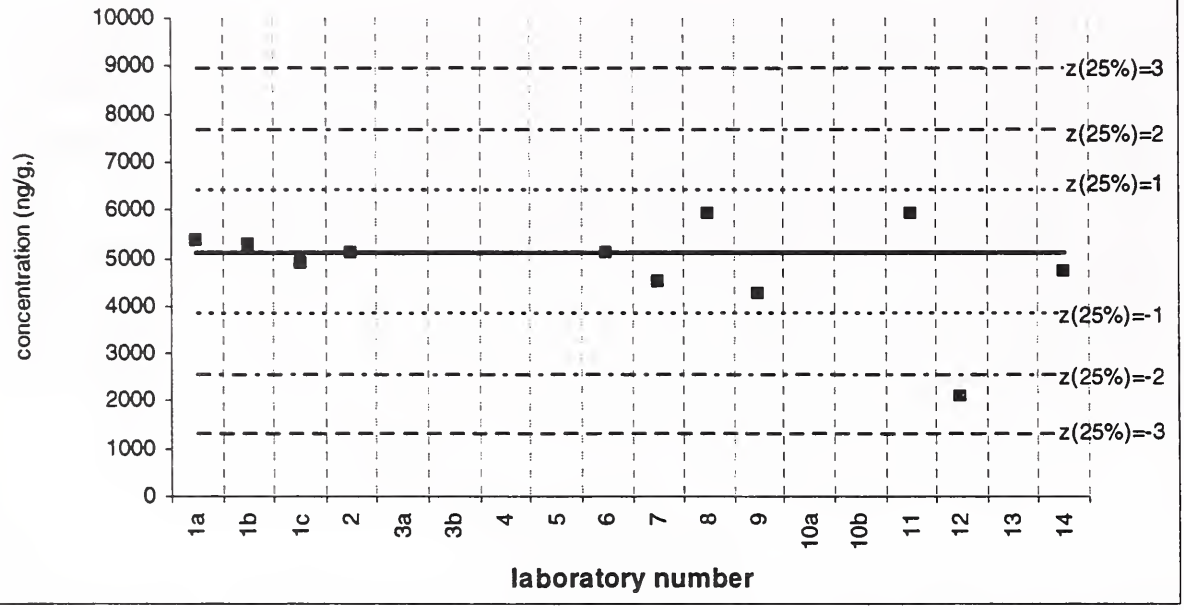


benzo[ghi]perylene

SRM 1648

Assigned value (solid line) = 5106 ng/g s = 555 ng/g 95% CL = 397 ng/g

Reported Results: 11 Quantitative Results: 11

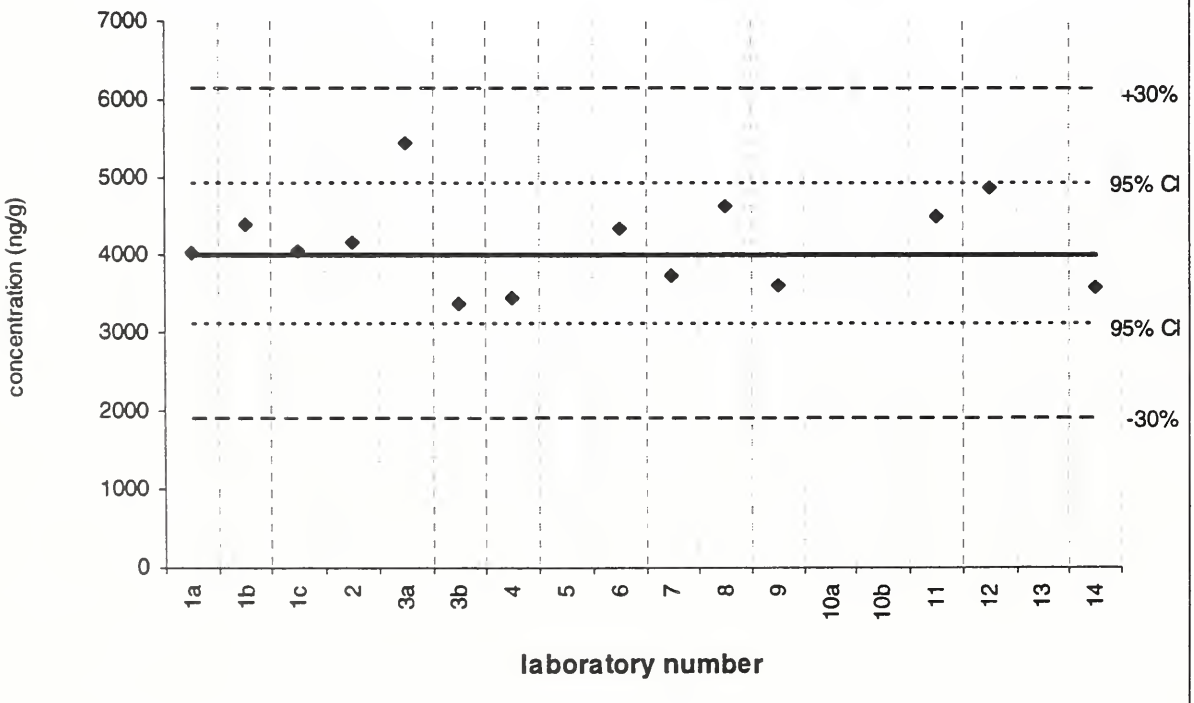


benzo[ghi]perylene

SRM 1649a

Certified Value (solid line) = 4010 ± 910 ng/g

Reported Results: 14 Quantitative Results: 14

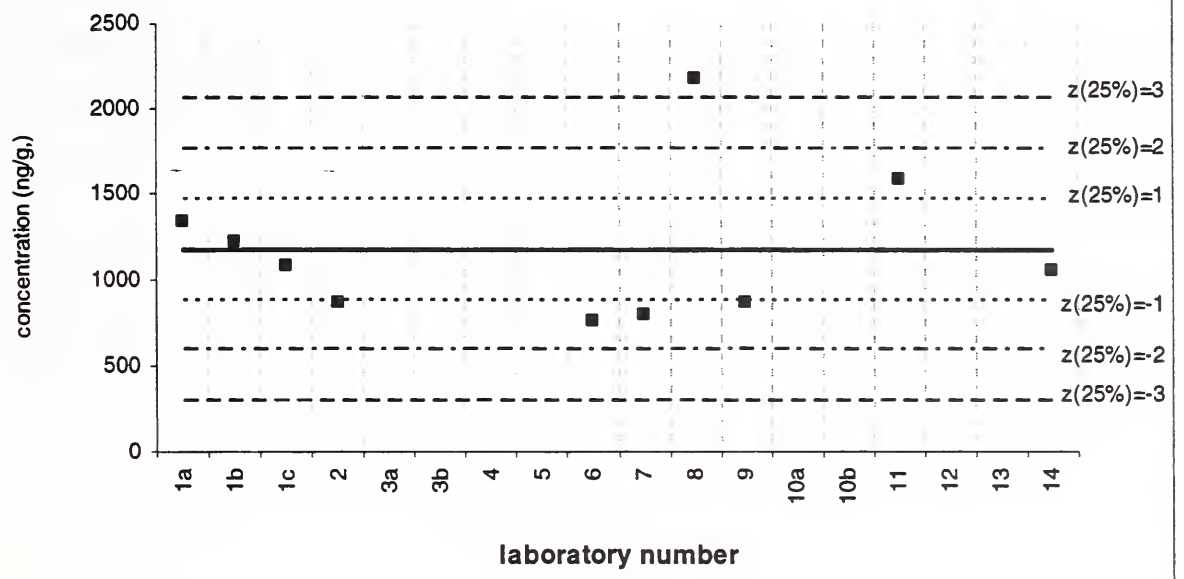


benzo[ghi]perylene

Baltimore 2 PM

Assigned value (solid line) = 1175 ng/g s = 440 ng/g 95% CL = 315 ng/g

Reported Results: 11 Quantitative Results: 10

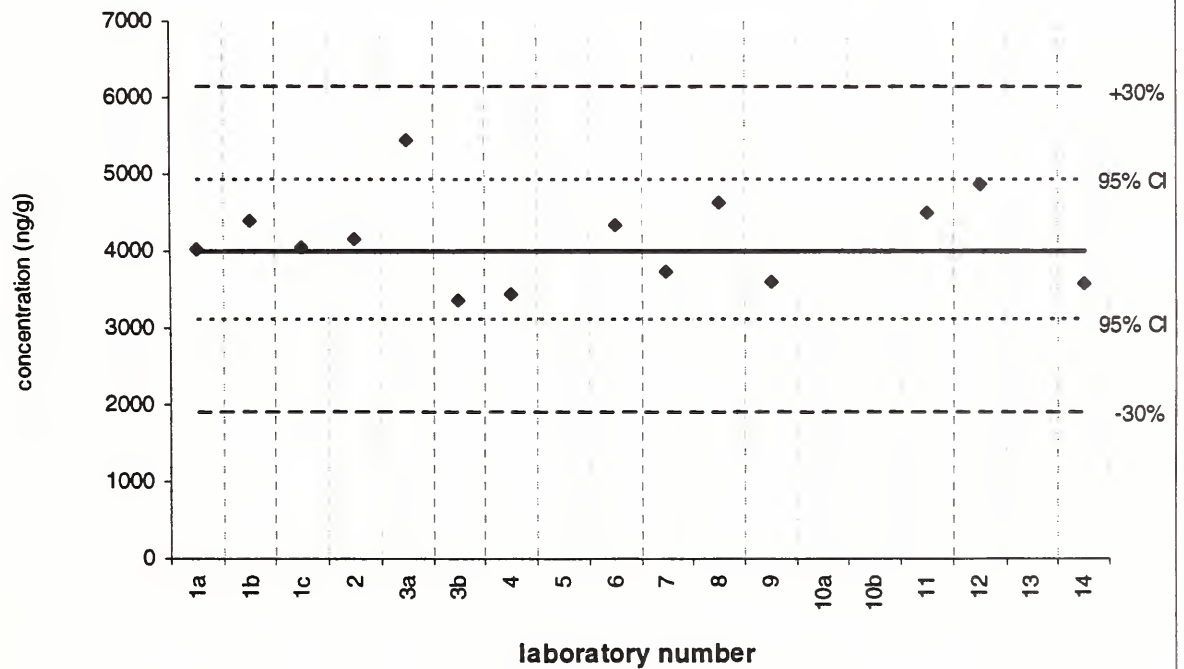


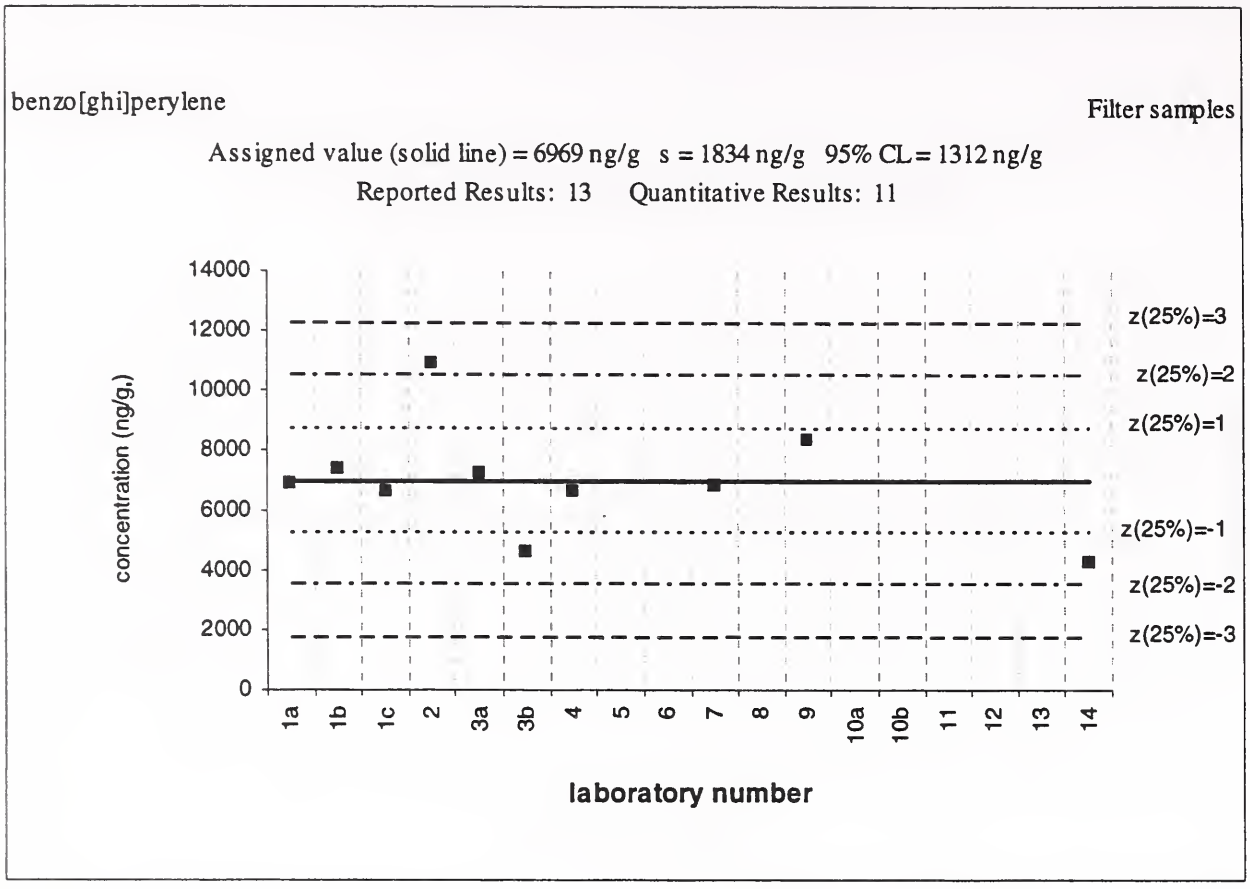
benzo[ghi]perylene

SRM 1649a

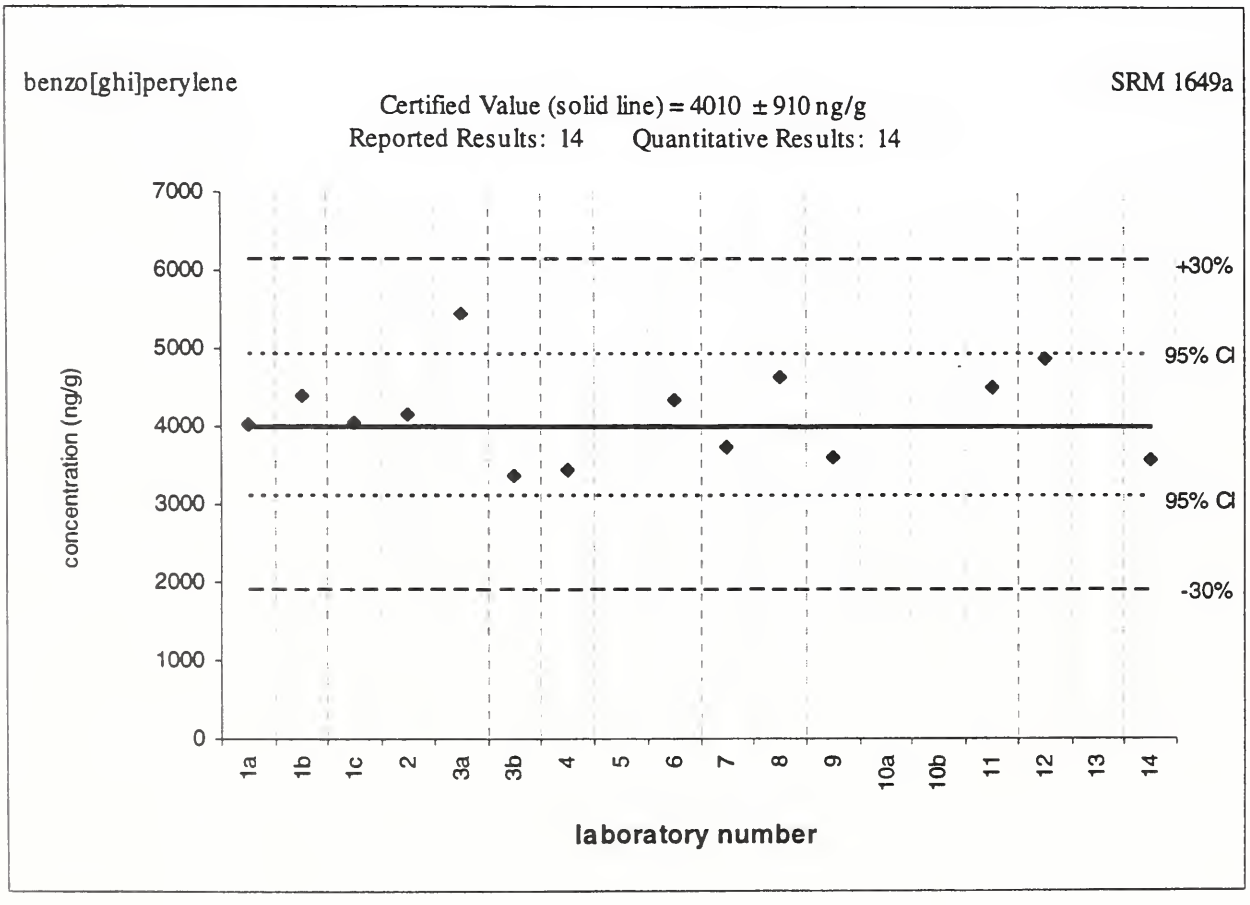
Certified Value (solid line) = 4010 ± 910 ng/g

Reported Results: 14 Quantitative Results: 14





lab 11 = 29886 ng/g

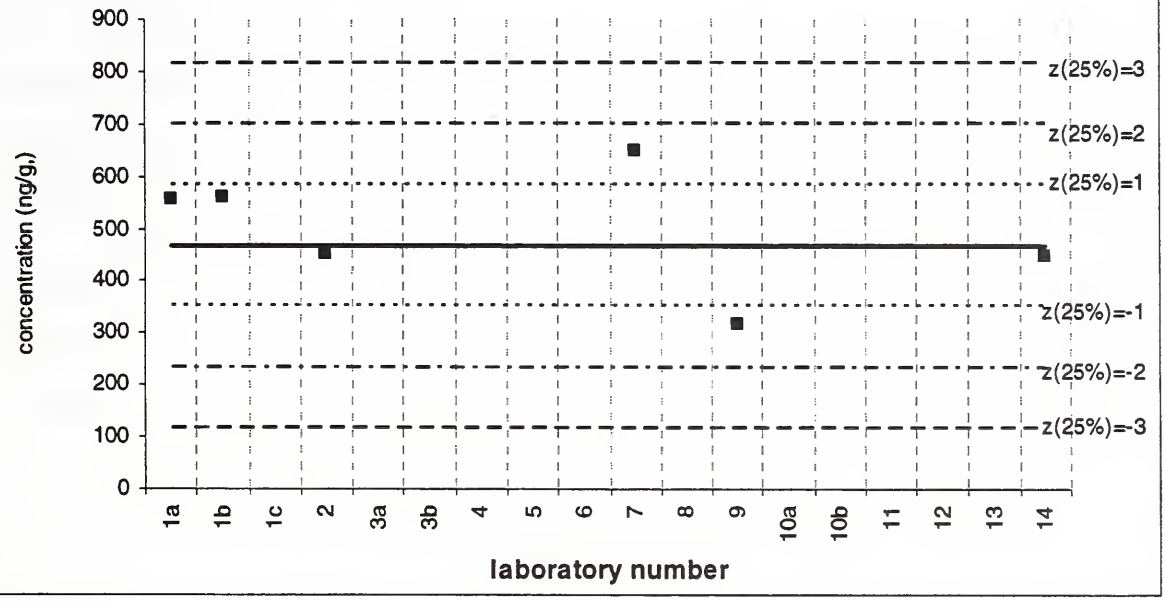


dibenz[a,h]anthracene

SRM 1648

Assigned value (solid line) = 467 ng/g s = 100 ng/g 95% CL = 124 ng/g

Reported Results: 7 Quantitative Results: 6

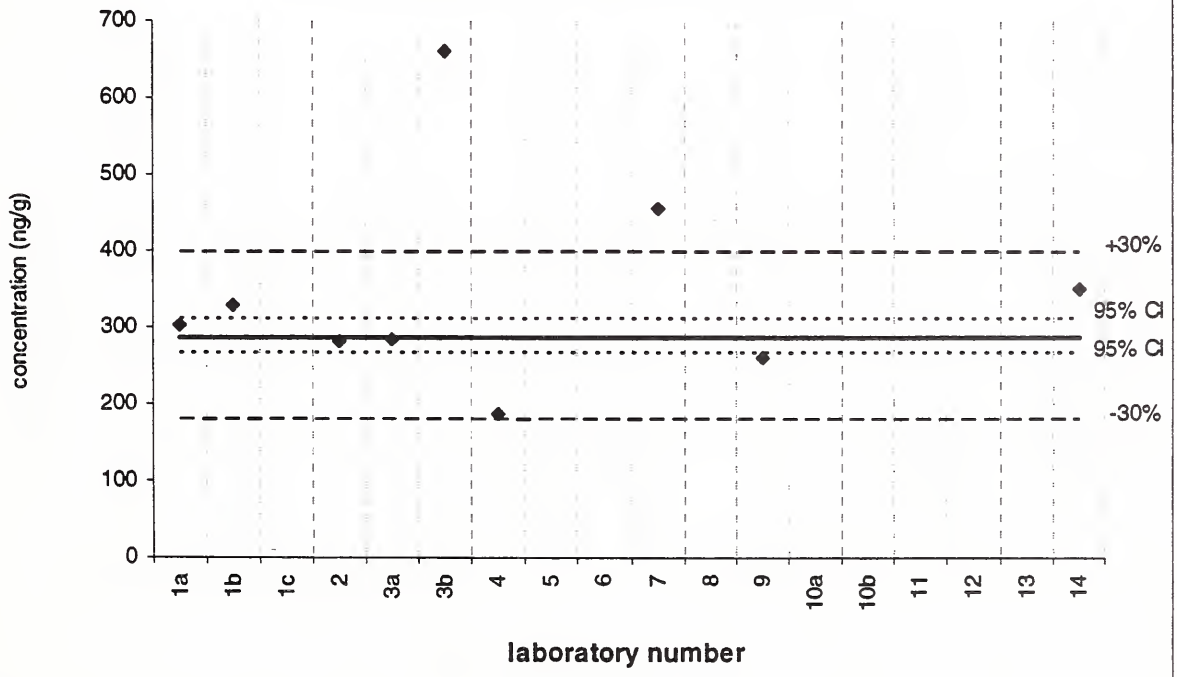


dibenz[a,h]anthracene

SRM 1649a

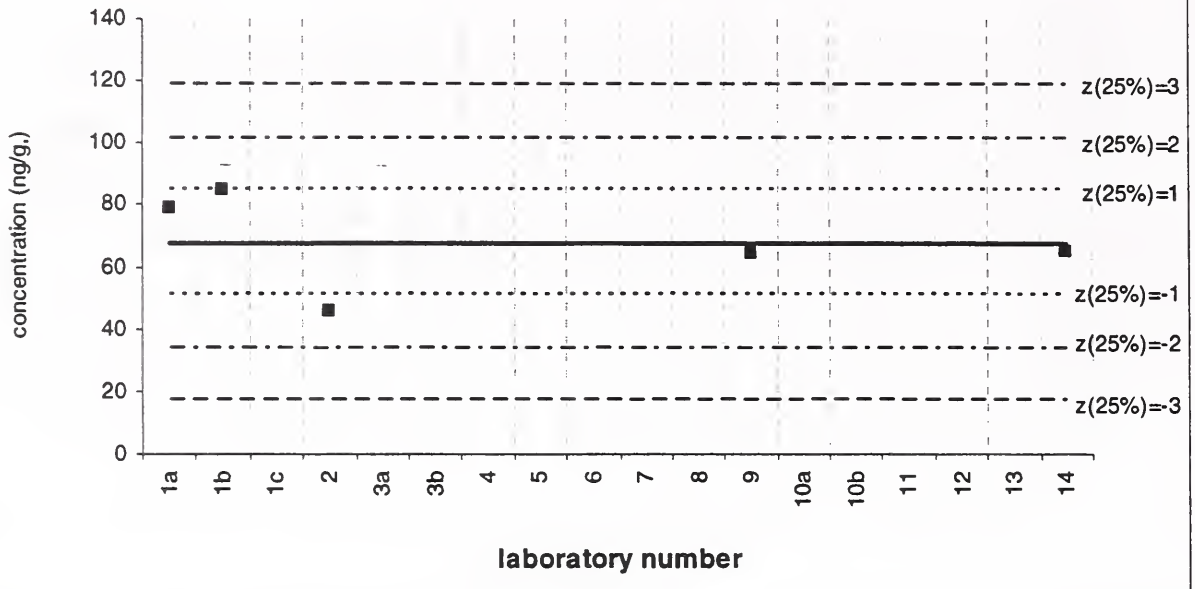
Certified Value (solid line) = 288 ± 23 ng/g

Reported Results: 10 Quantitative Results: 9



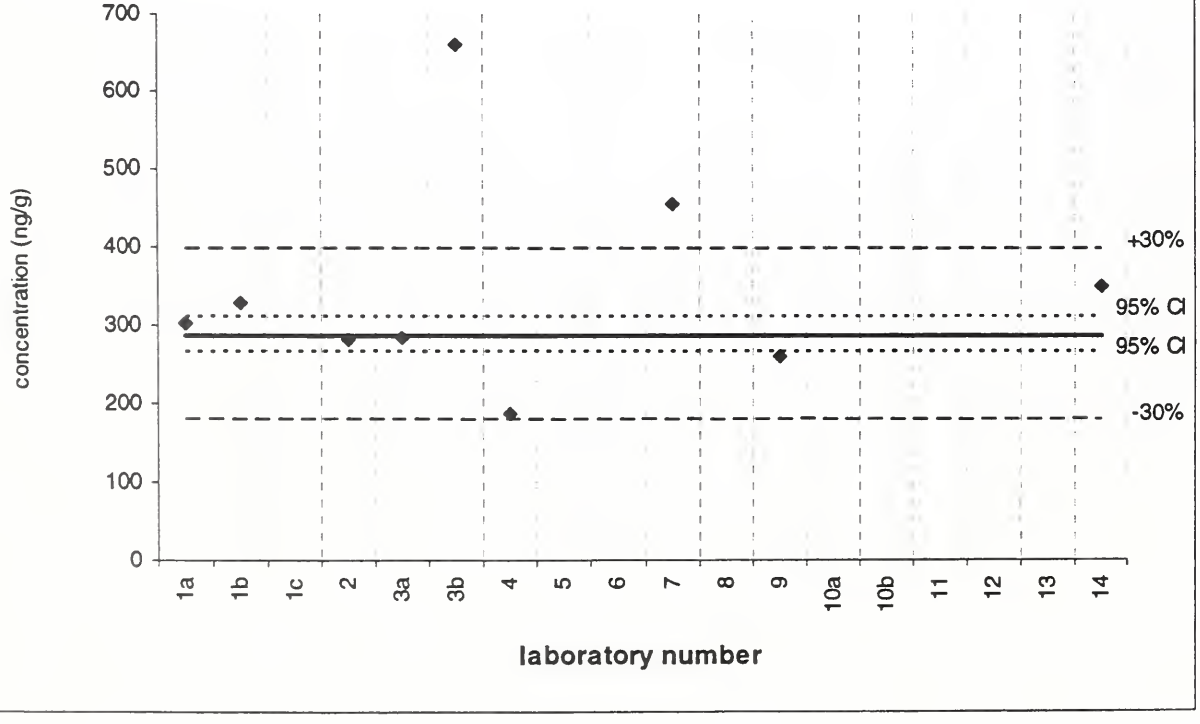
dibenz[a,h]anthracene Baltimore 2 PM

Assigned value (solid line) = 67.7 ng/g s = 15.2 ng/g 95% CL = 18.9 ng/g
Reported Results: 7 Quantitative Results: 5



dibenz[a,h]anthracene SRM 1649a

Certified Value (solid line) = 288 ± 23 ng/g
Reported Results: 10 Quantitative Results: 9

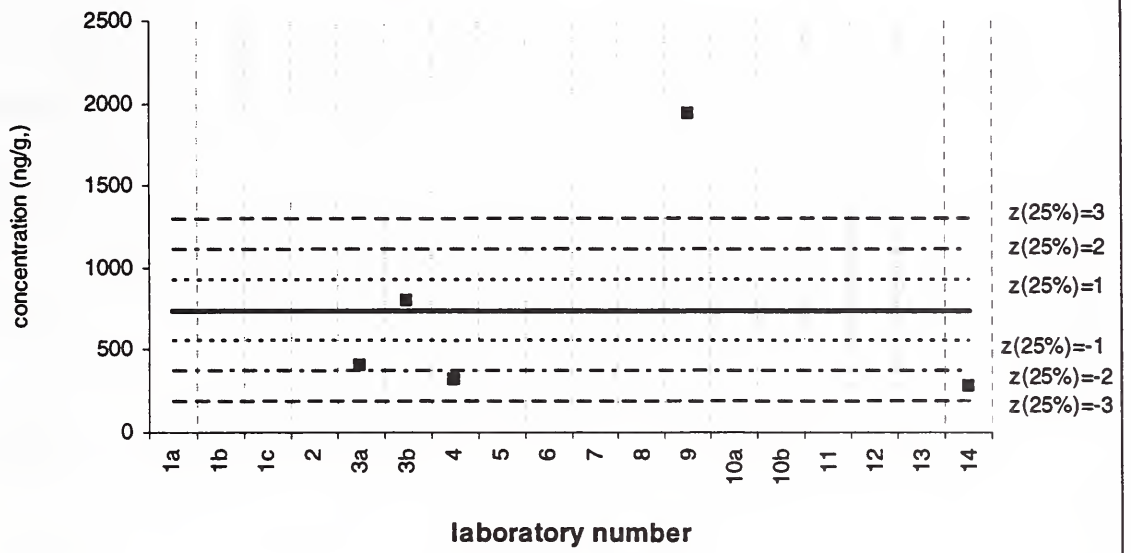


dibenz[a,h]anthracene

Filter samples

Assigned value (solid line) = 738 ng/g s = 803 ng/g 95% CL = 1277 ng/g

Reported Results: 10 Quantitative Results: 5

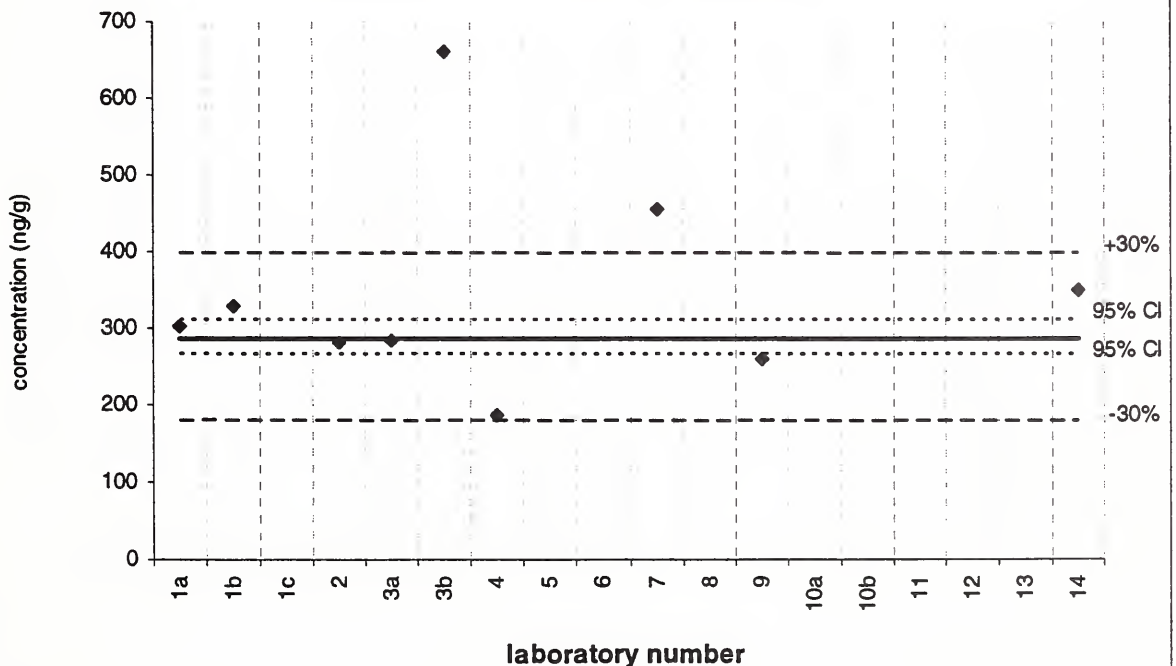


dibenz[a,h]anthracene

SRM 1649a

Certified Value (solid line) = 288 ± 23 ng/g

Reported Results: 10 Quantitative Results: 9

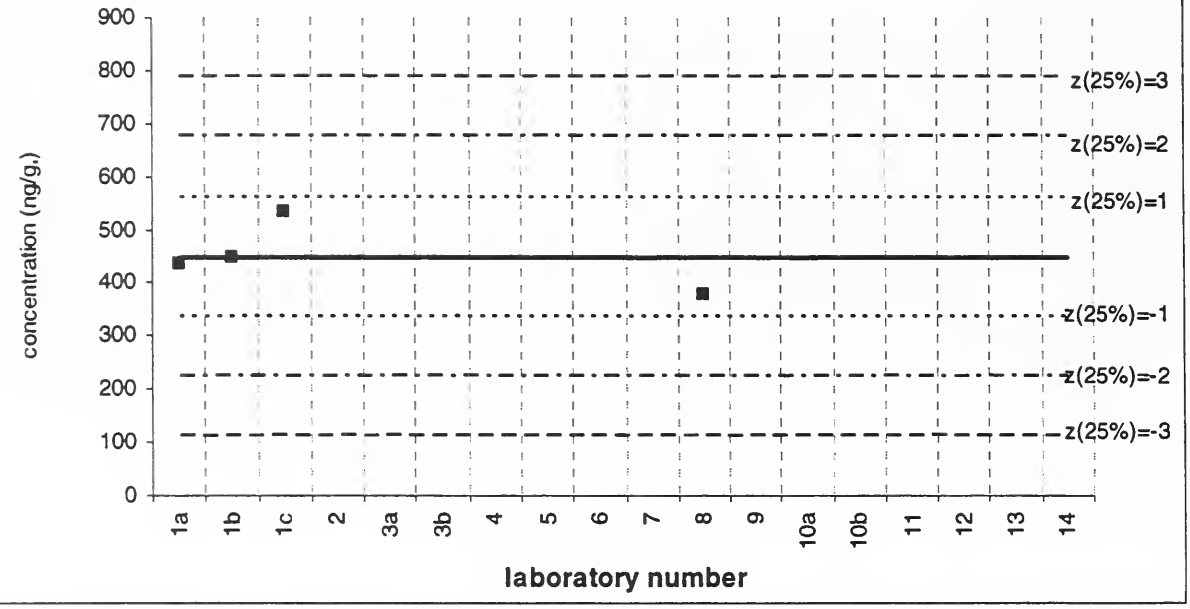


dibenz[a,c]anthracene

SRM 1648

Assigned value (solid line) = 450 ng/g s = 65 ng/g 95% CL = 104 ng/g

Reported Results: 5 Quantitative Results: 4

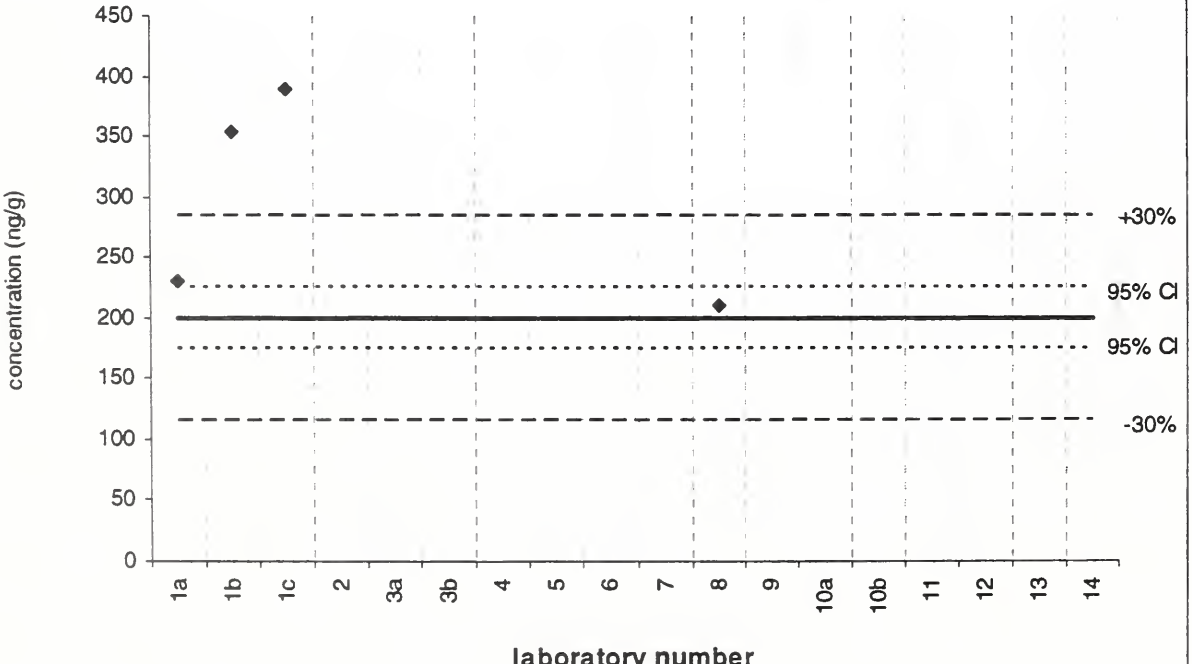


dibenz[a,c]anthracene

SRM 1649a

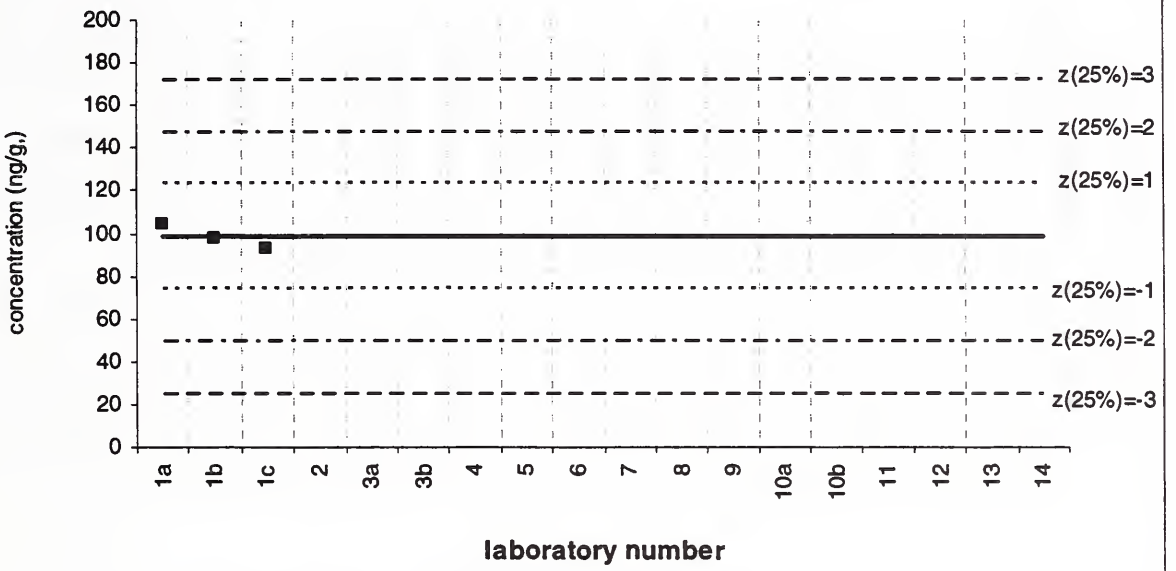
Certified Value (solid line) = 200 ± 25 ng/g

Reported Results: 5 Quantitative Results: 4



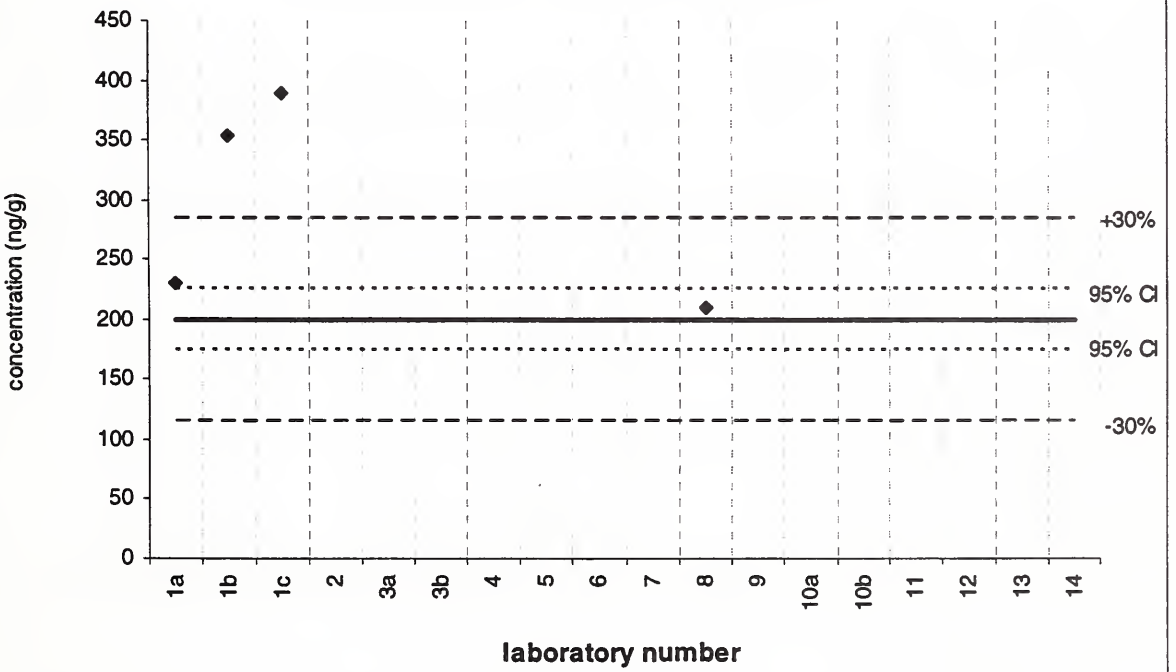
dibenz[a,c]anthracene Baltimore 2 PM

Assigned value (solid line) = 98.2 ng/g s = 5.8 ng/g 95% CL = 14.3 ng/g
Reported Results: 5 Quantitative Results: 3



dibenz[a,c]anthracene SRM 1649a

Certified Value (solid line) = 200 ± 25 ng/g
Reported Results: 5 Quantitative Results: 4

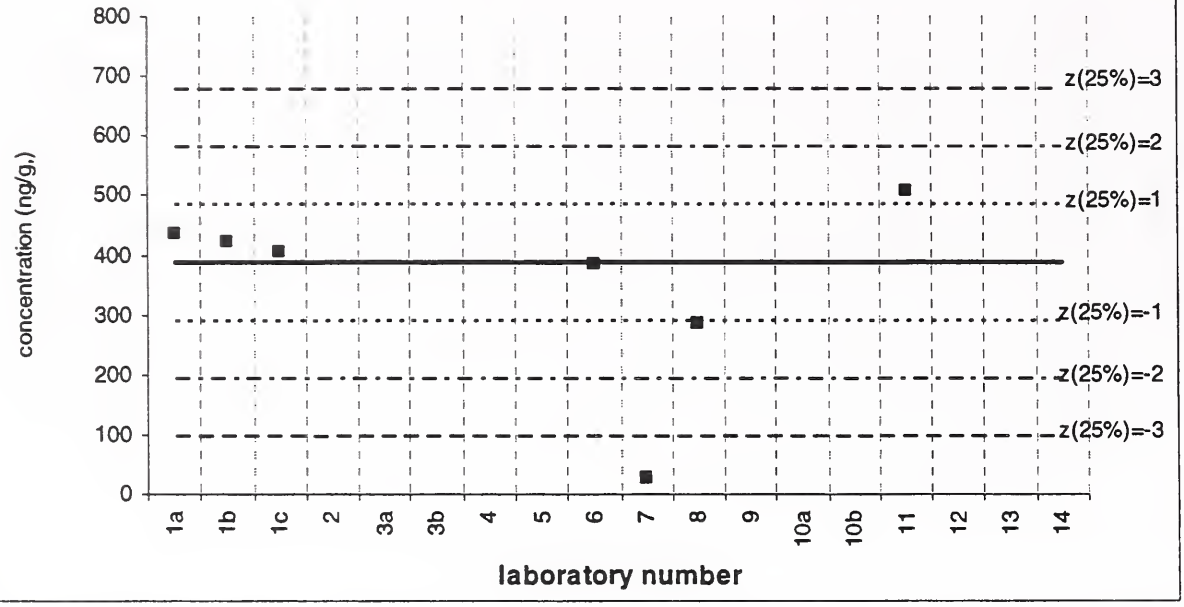


benzo[b]chrysene

SRM 1648

Assigned value (solid line) = 386 ng/g s = 61 ng/g 95% CL = 75 ng/g

Reported Results: 8 Quantitative Results: 7

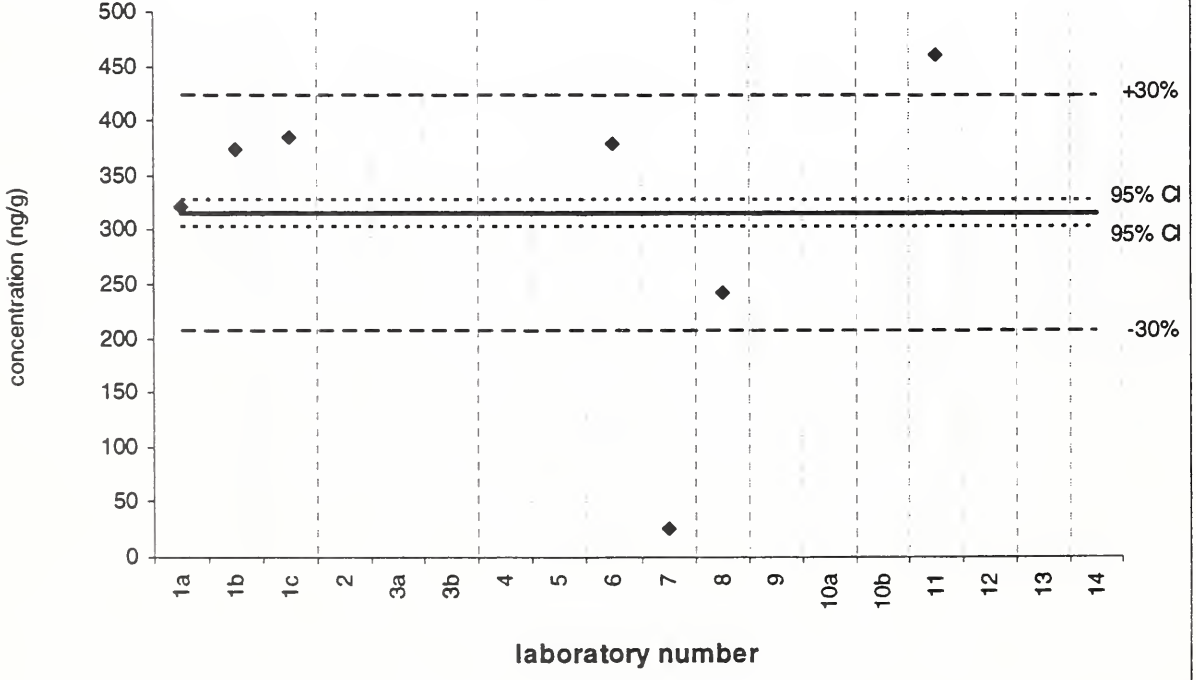


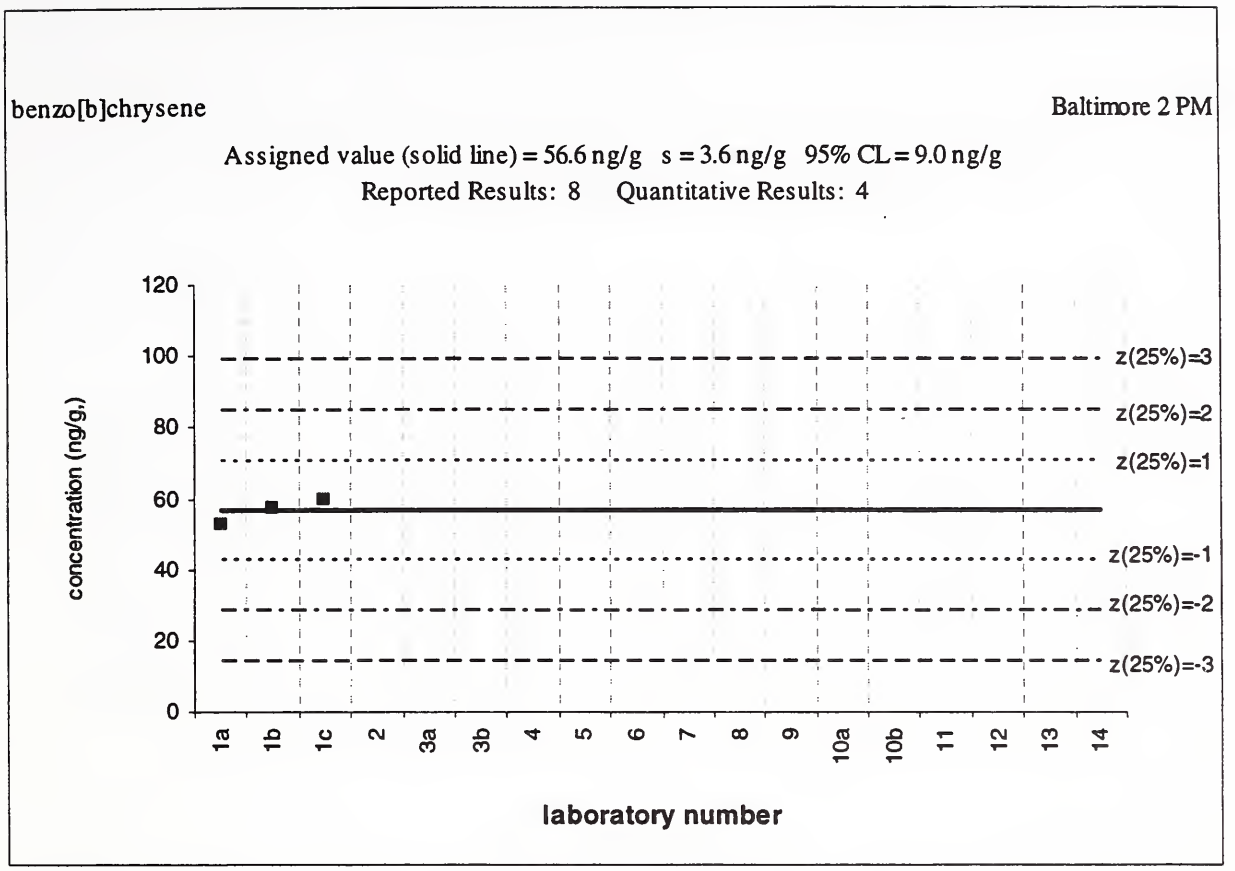
benzo[b]chrysene

SRM 1649a

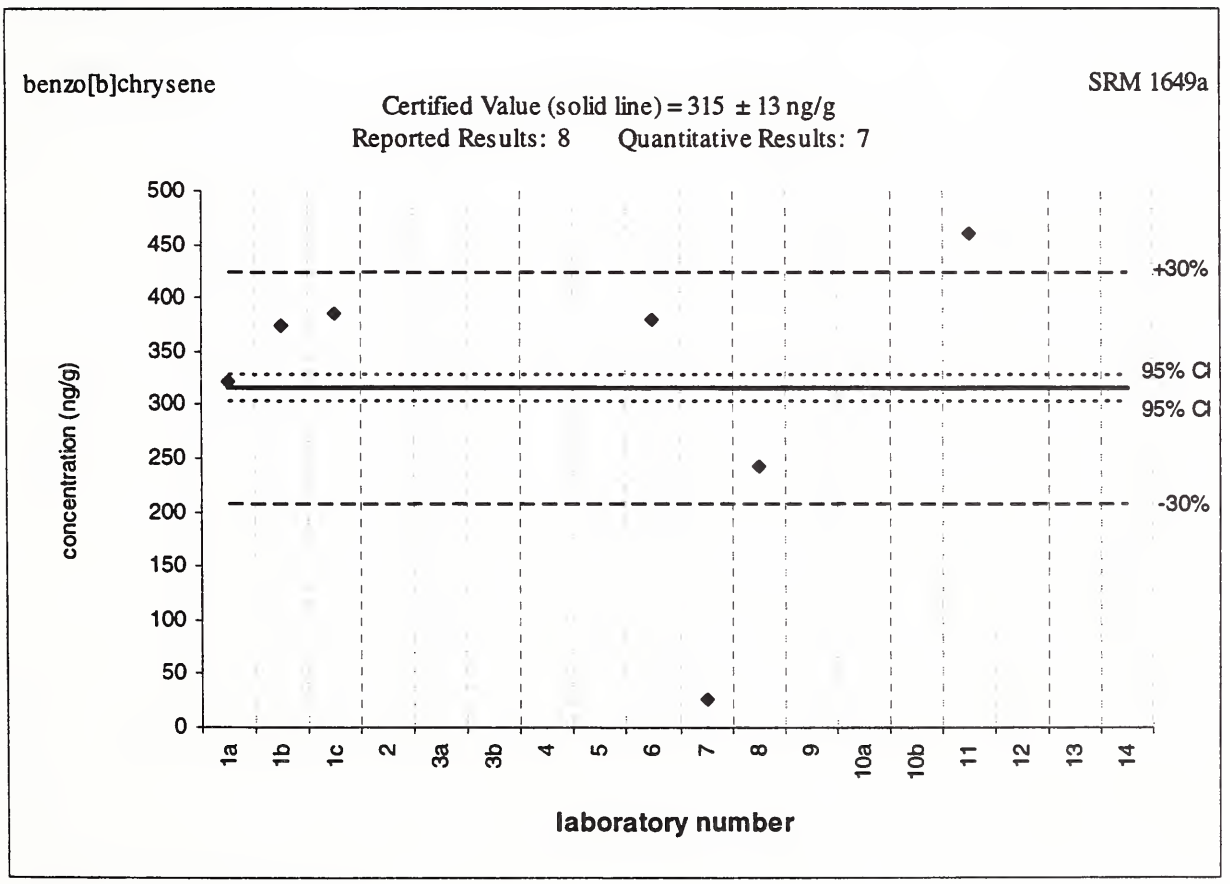
Certified Value (solid line) = 315 ± 13 ng/g

Reported Results: 8 Quantitative Results: 7





lab 11 = 490 ng/g

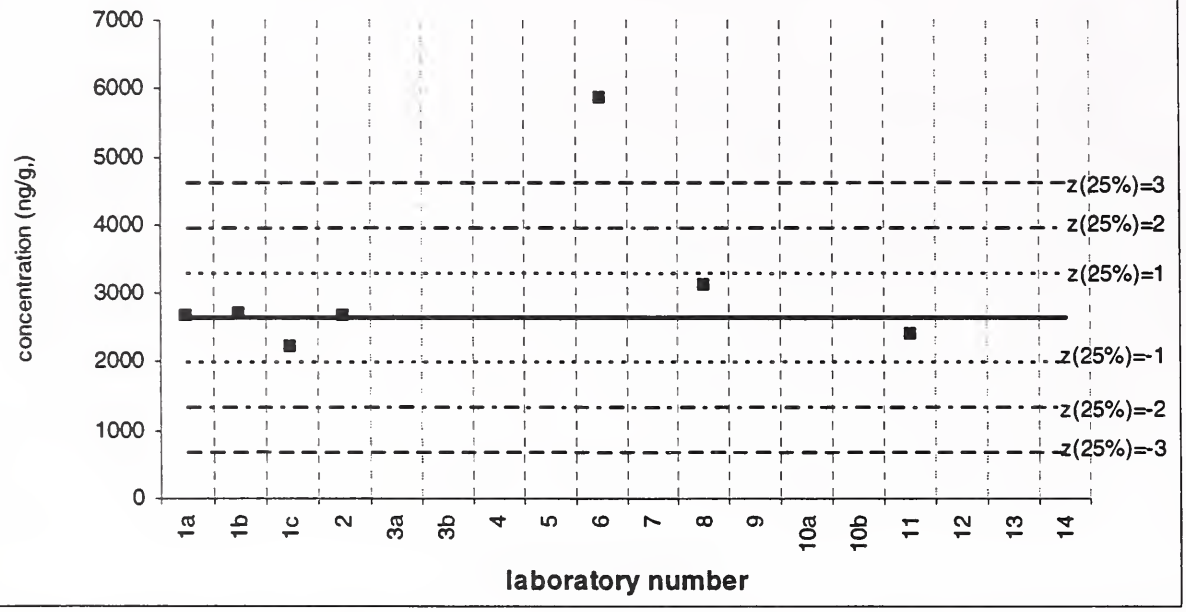


coronene

SRM 1648

Assigned value (solid line) = 2632 ng/g s = 306 ng/g 95% CL = 321 ng/g

Reported Results: 8 Quantitative Results: 7

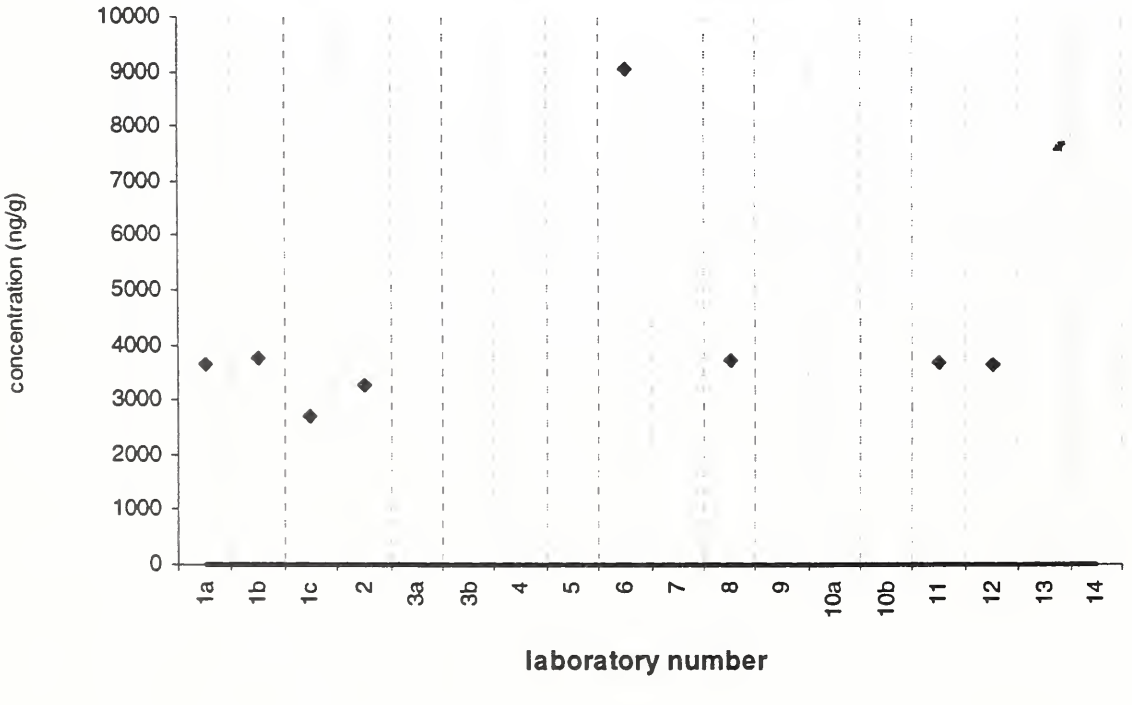


coronene

SRM 1649a

Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 8

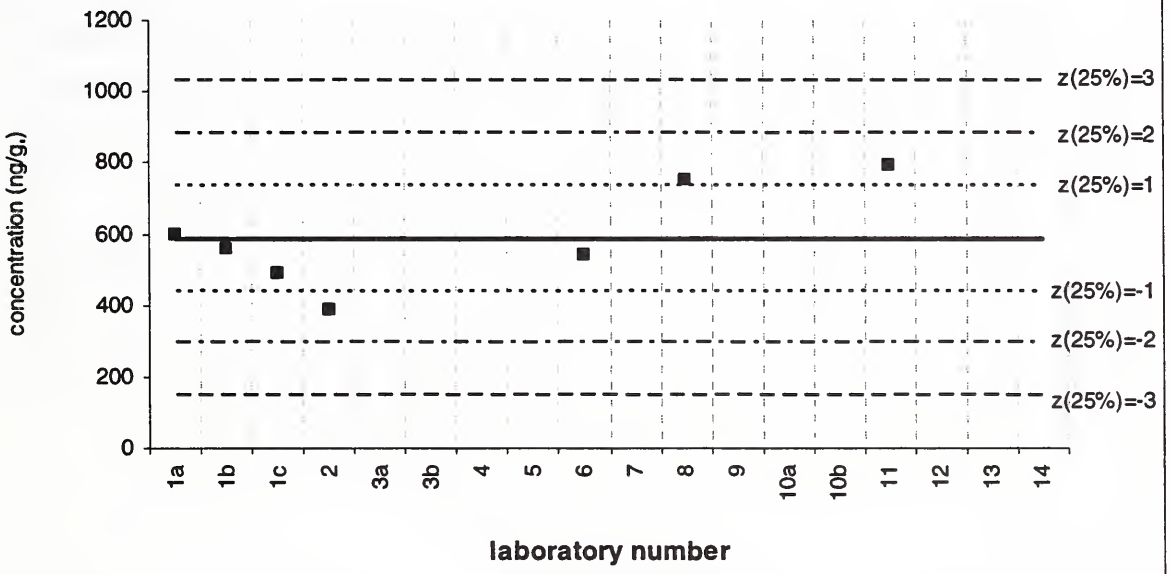


coronene

Baltimore 2 PM

Assigned value (solid line) = 587 ng/g s = 142 ng/g 95% CL = 131 ng/g

Reported Results: 9 Quantitative Results: 7

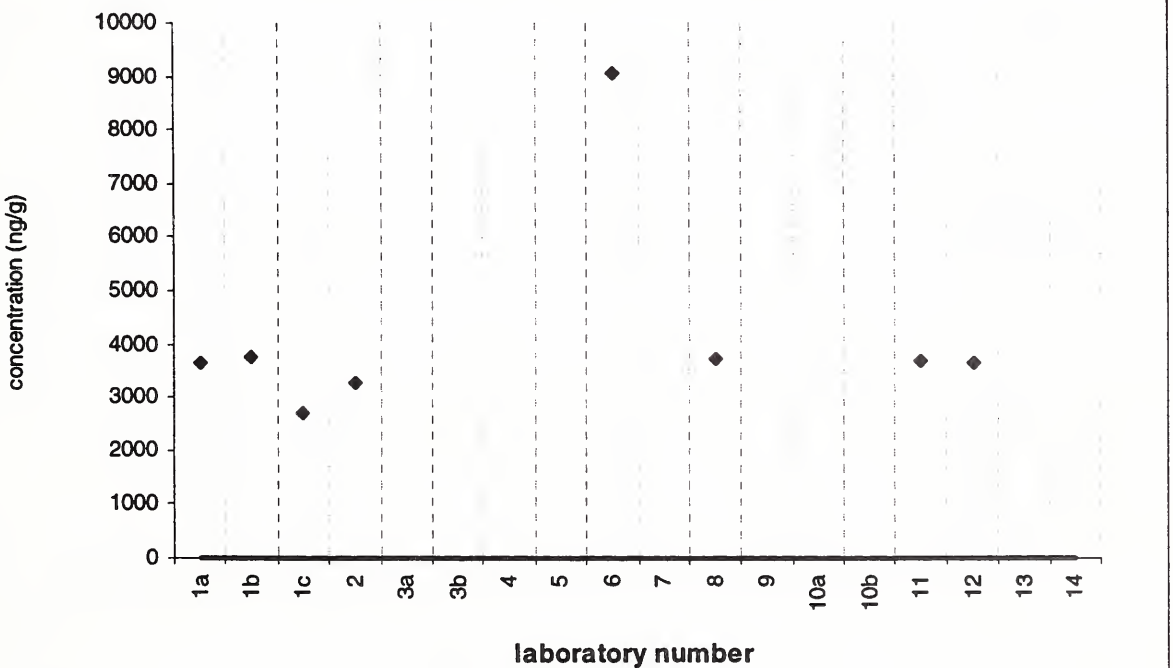


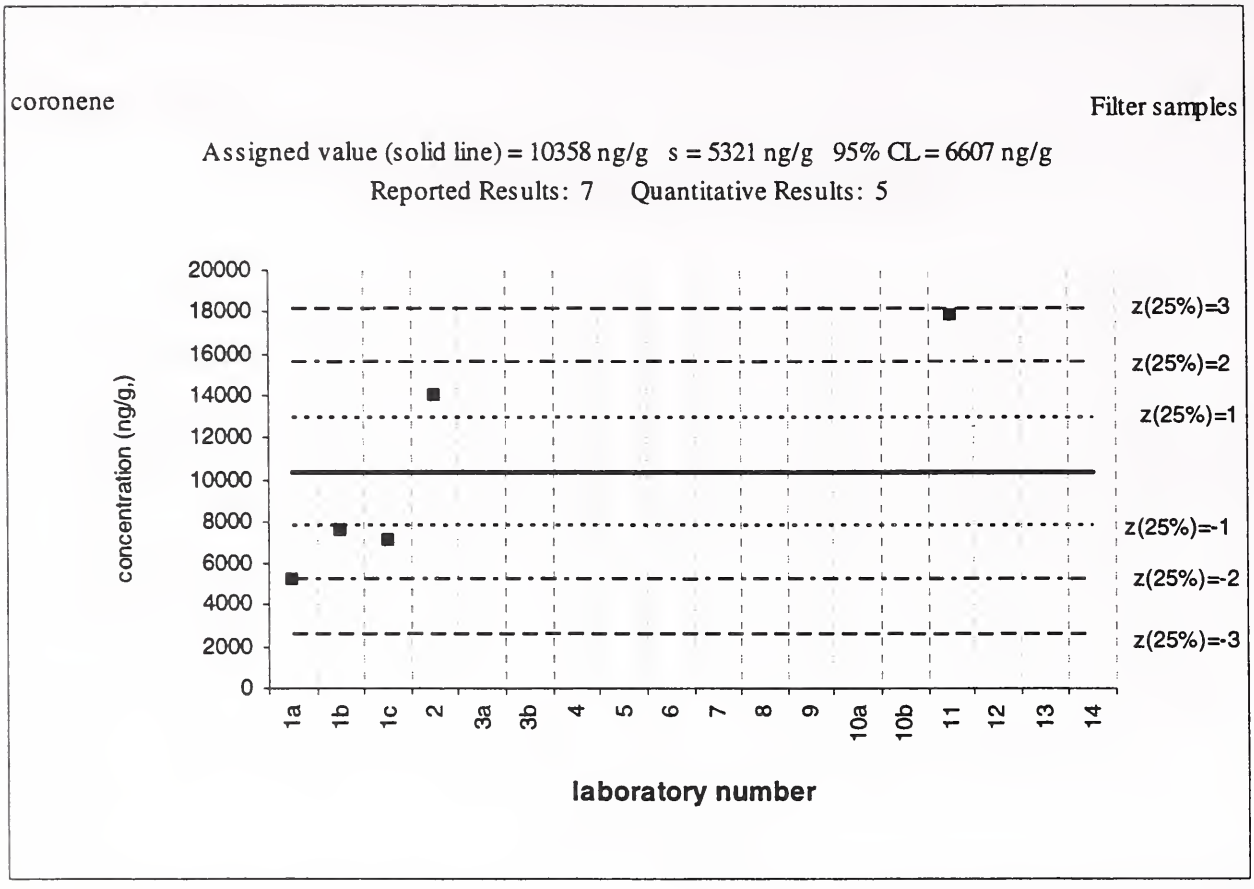
coronene

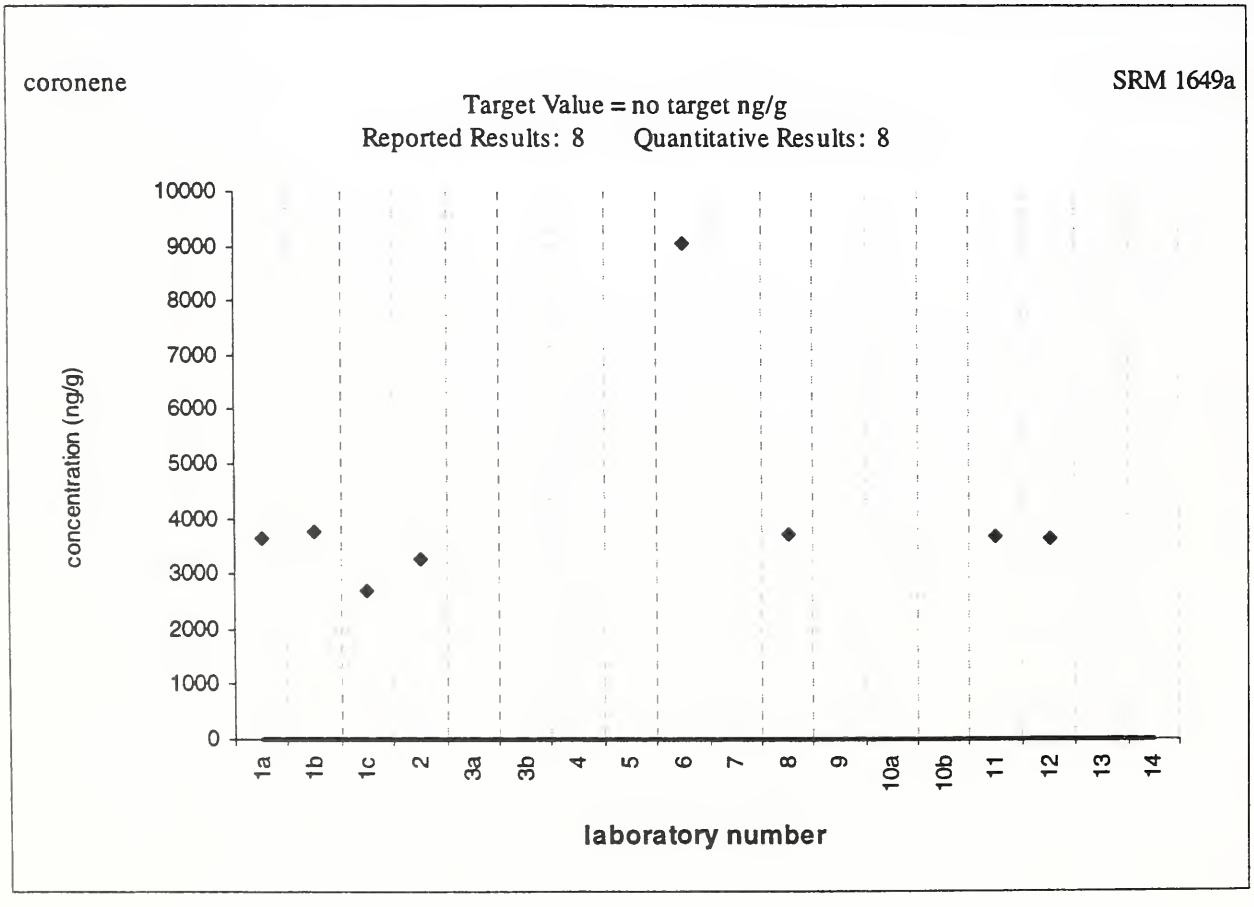
SRM 1649a

Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 8




coronene
Filter samples
Assigned value (solid line) = 10358 ng/g s = 5321 ng/g 95% CL = 6607 ng/g
Reported Results: 7 Quantitative Results: 5
concentration (ng/g)
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

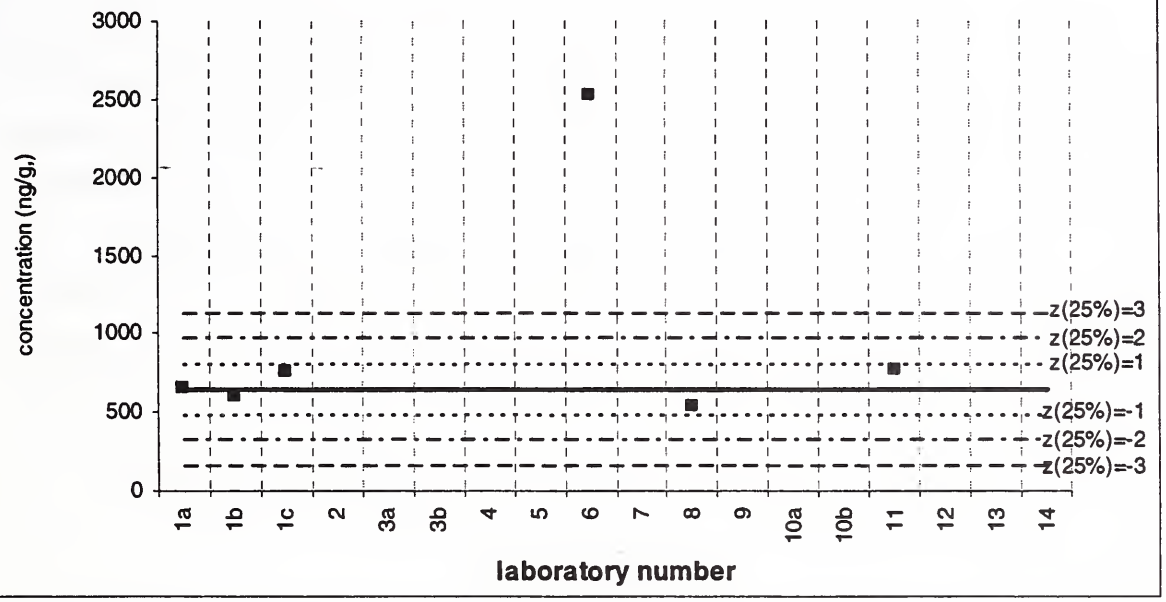

coronene
SRM 1649a
Target Value = no target ng/g
Reported Results: 8 Quantitative Results: 8
concentration (ng/g)
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

dibenzo[a,e]pyrene

SRM 1648

Assigned value (solid line) = 640 ng/g s = 92 ng/g 95% CL = 146 ng/g

Reported Results: 7 Quantitative Results: 6

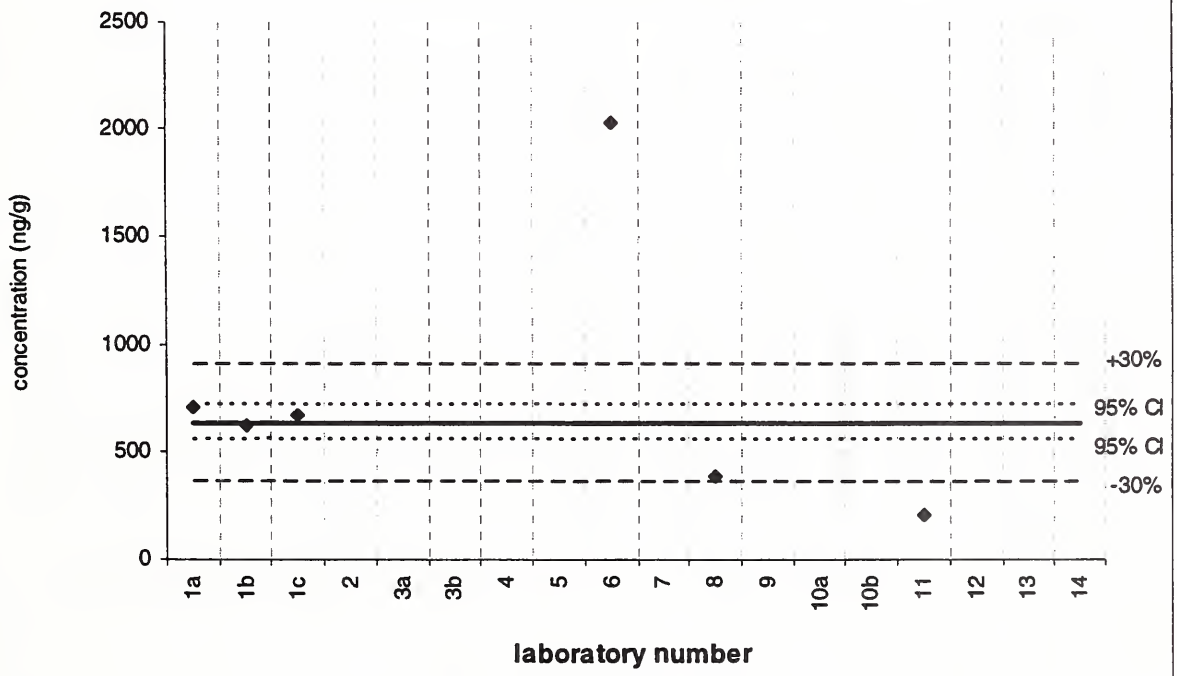


dibenzo[a,e]pyrene

SRM 1649a

Reference Value (solid line) = 630 ± 80 ng/g

Reported Results: 7 Quantitative Results: 6

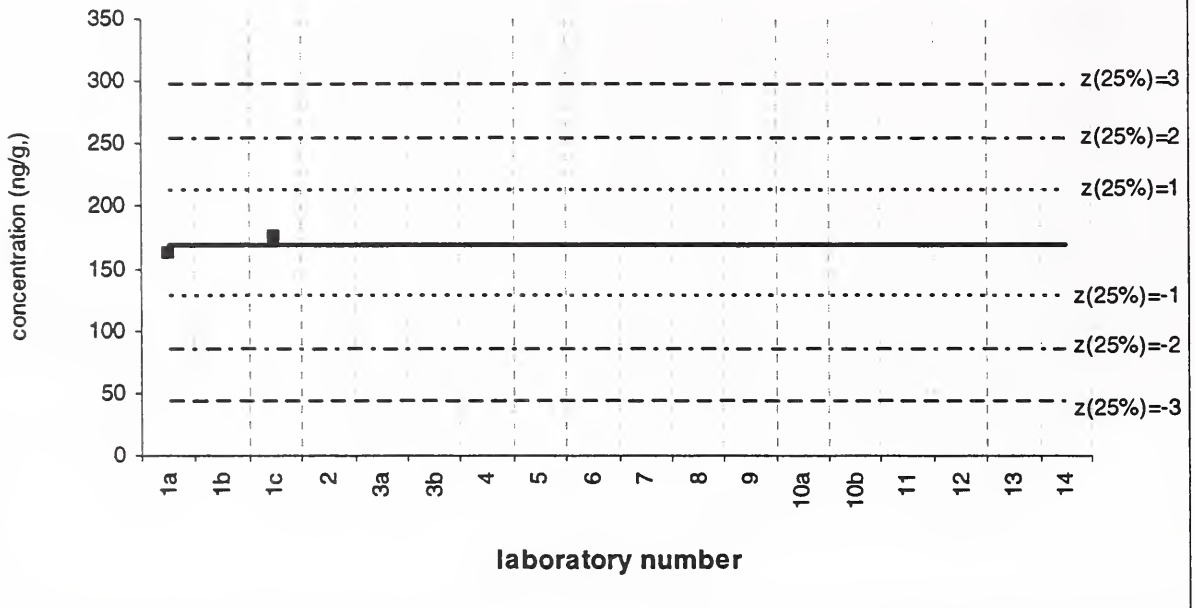


dibenzo[a,e]pyrene

Baltimore 2 PM

Assigned value (solid line) = 170 ng/g s = 9 ng/g 95% CL = 85 ng/g

Reported Results: 7 Quantitative Results: 2

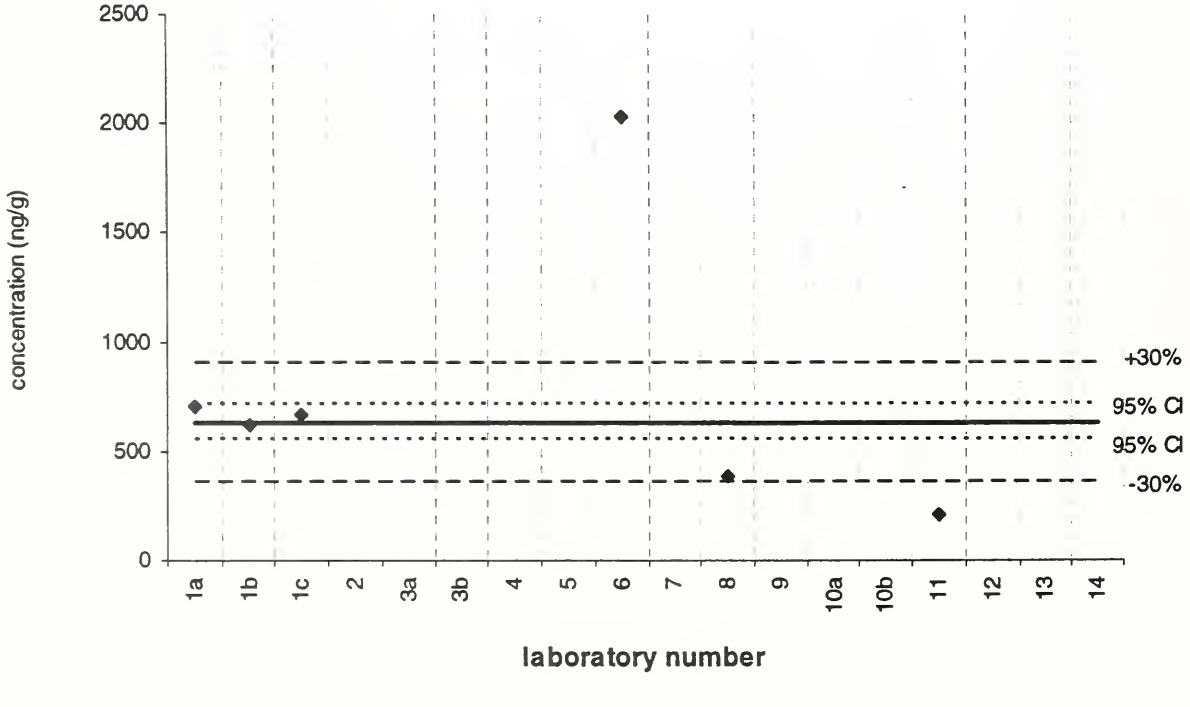


dibenzo[a,e]pyrene

SRM 1649a

Reference Value (solid line) = 630 ± 80 ng/g

Reported Results: 7 Quantitative Results: 6

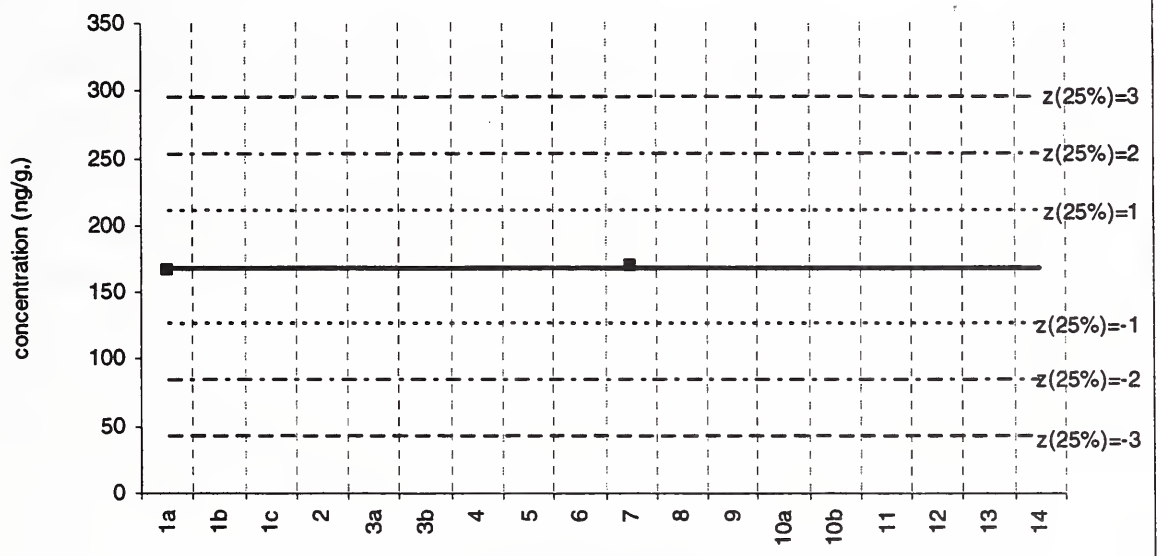


9-nitroanthracene

SRM 1648

Assigned value (solid line) = 168 ng/g s = 1 ng/g 95% CL = 11 ng/g

Reported Results: 2 Quantitative Results: 2

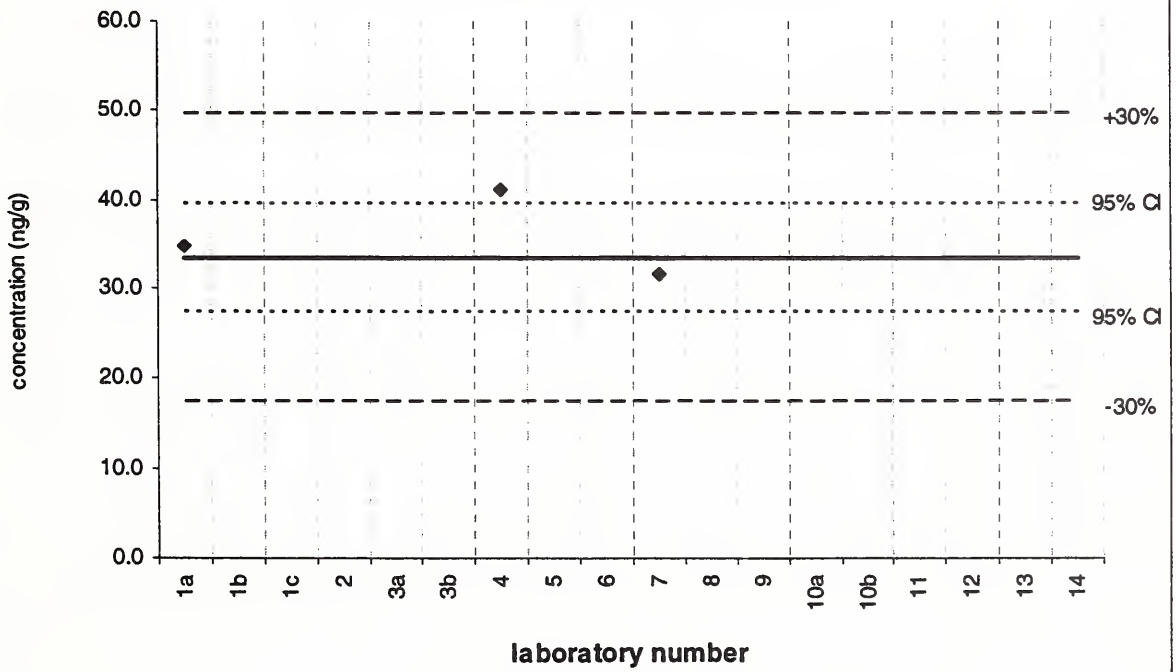


9-nitroanthracene

SRM 1649a

Target Value (solid line) = 33.4 ± 6.1 ng/g

Reported Results: 3 Quantitative Results: 3

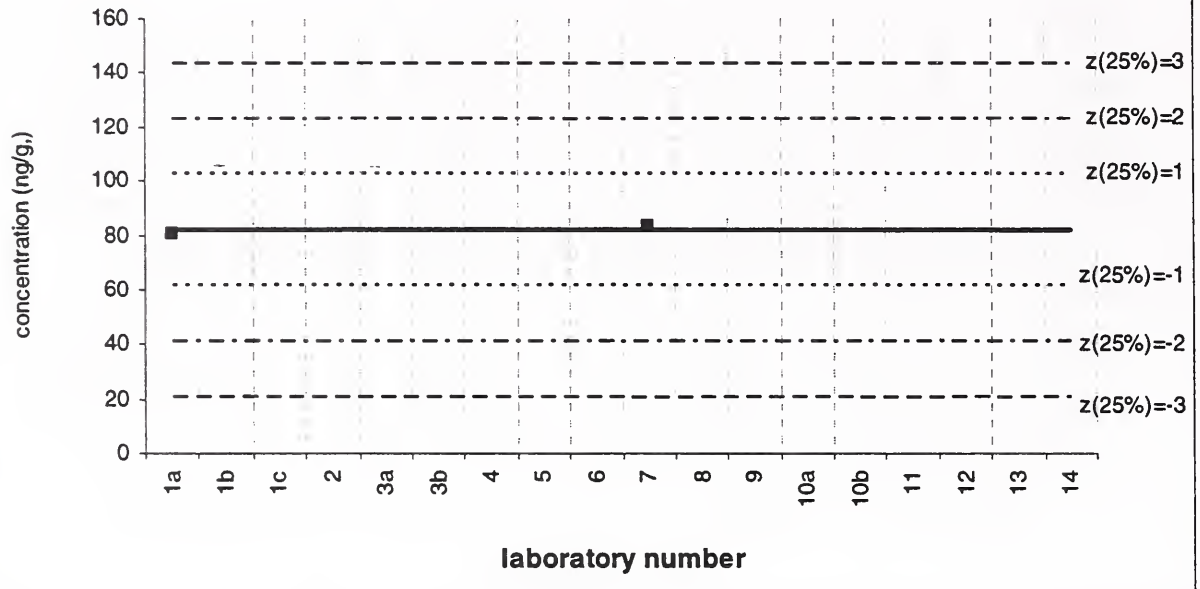


9-nitroanthracene

Baltimore 2 PM

Assigned value (solid line) = 81.9 ng/g s = 2.2 ng/g 95% CL = 19.7 ng/g

Reported Results: 2 Quantitative Results: 2

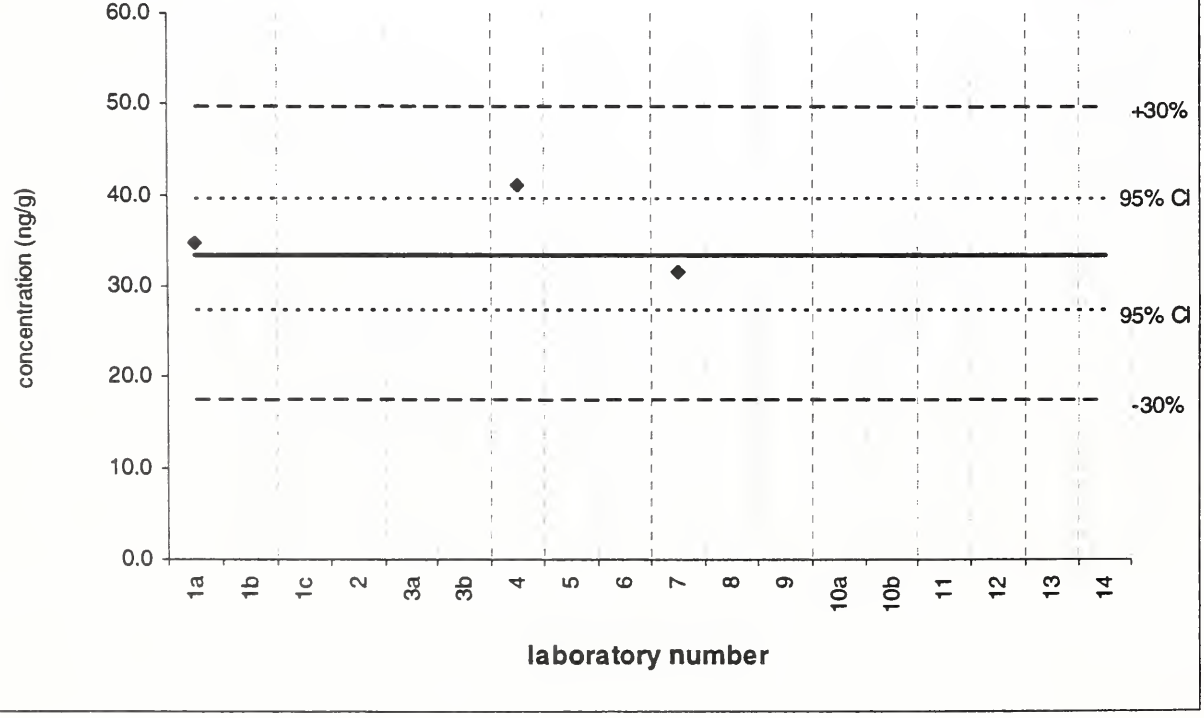


9-nitroanthracene

SRM 1649a

Target Value (solid line) = 33.4 ± 6.1 ng/g

Reported Results: 3 Quantitative Results: 3

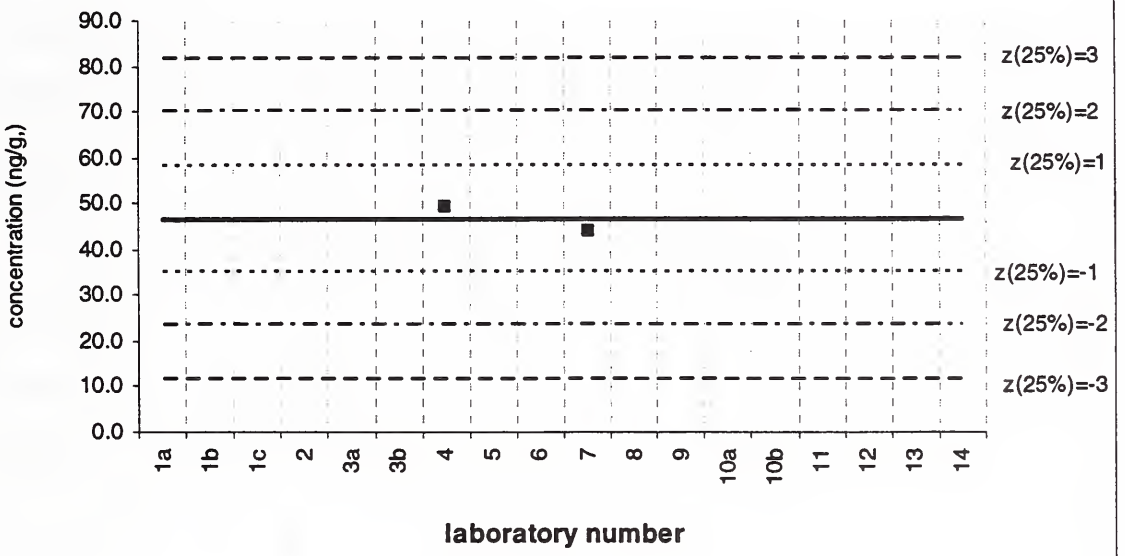


9-nitroanthracene

Filter samples

Assigned value (solid line) = 46.6 ng/g s = 3.7 ng/g 95% CL = 33.7 ng/g

Reported Results: 3 Quantitative Results: 2

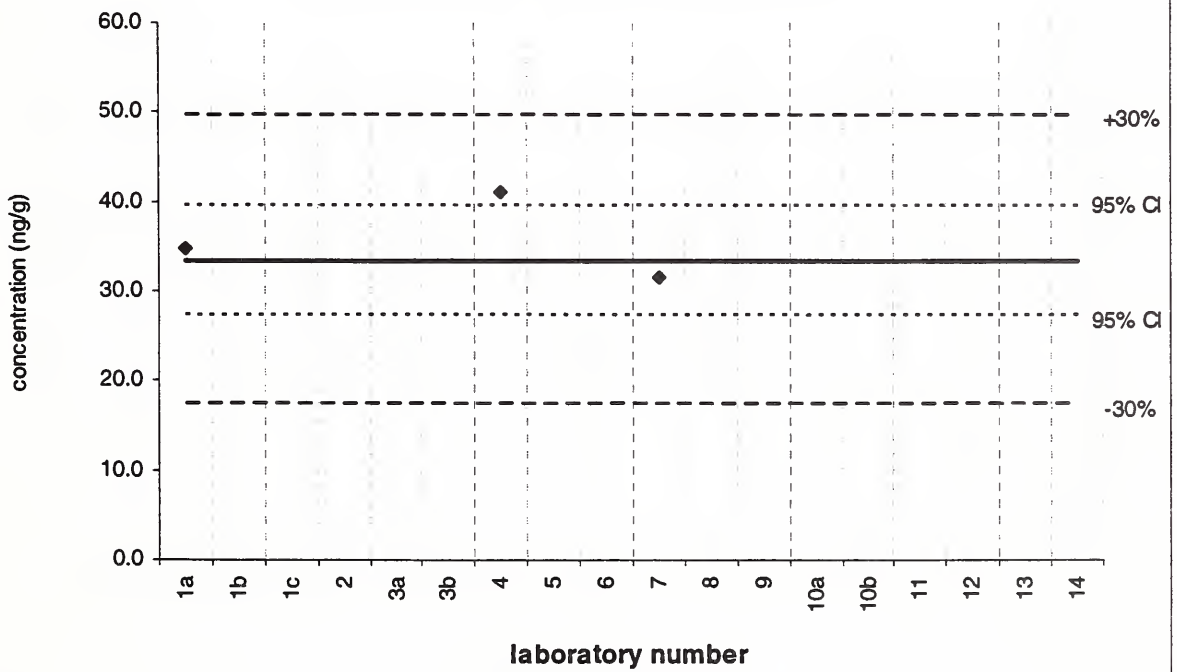


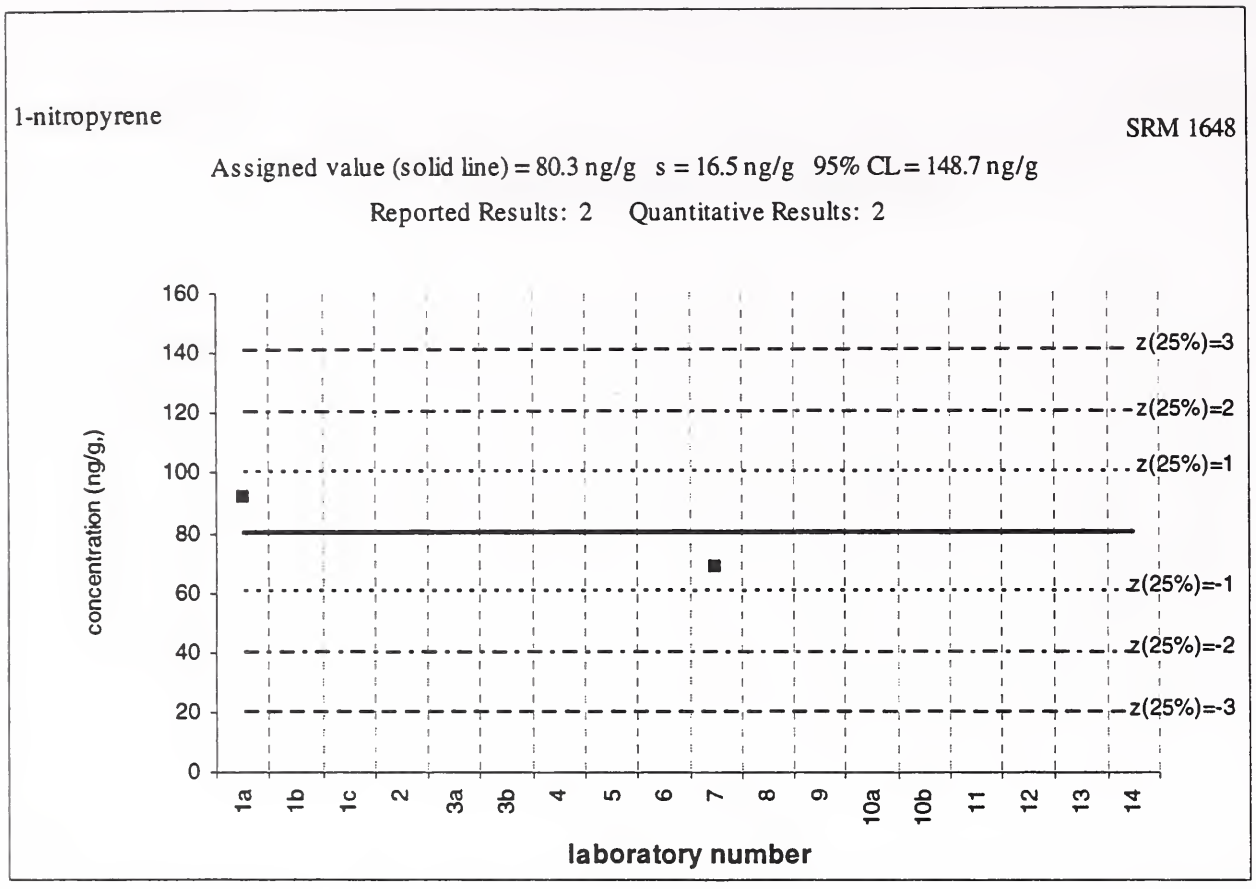
9-nitroanthracene

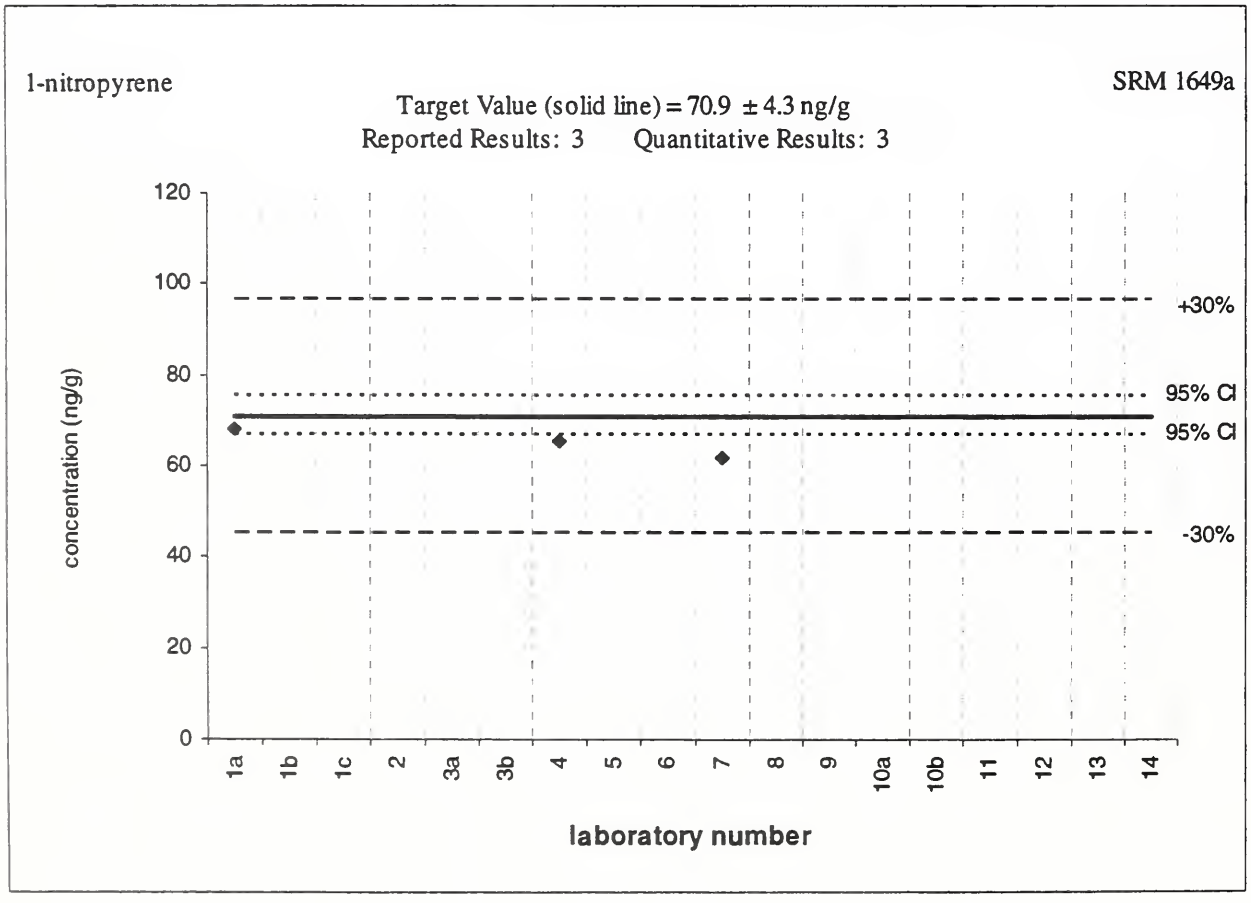
SRM 1649a

Target Value (solid line) = 33.4 ± 6.1 ng/g

Reported Results: 3 Quantitative Results: 3




1-nitropyrene
SRM 1648
Assigned value (solid line) = 80.3 ng/g s = 16.5 ng/g 95% CL = 148.7 ng/g
Reported Results: 2 Quantitative Results: 2
concentration (ng/g)
160
140
120
100
80
60
40
20
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

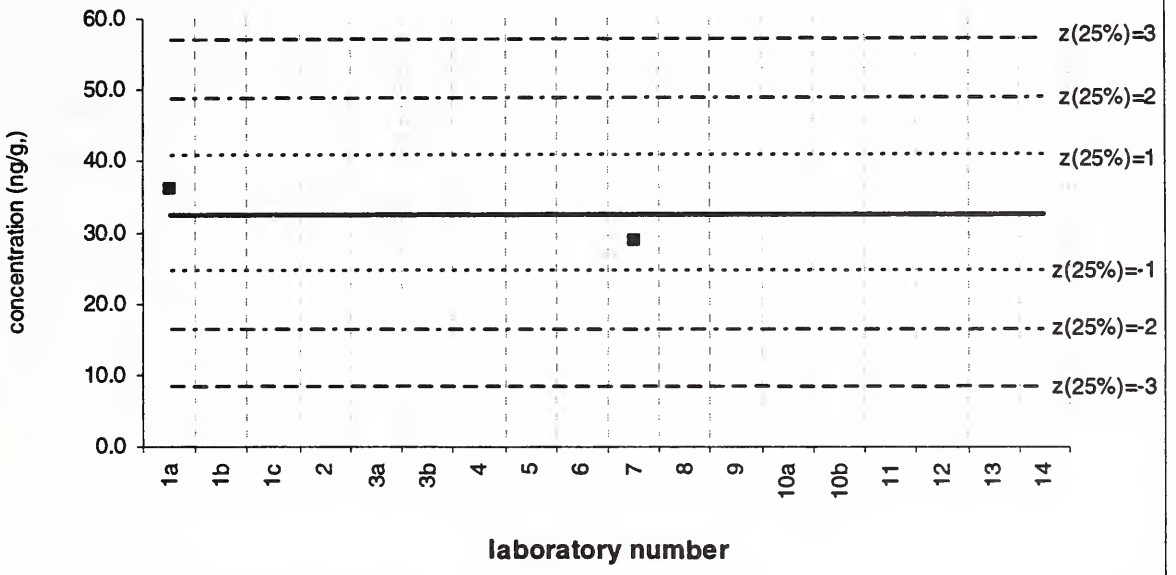

1-nitropyrene
SRM 1649a
Target Value (solid line) = 70.9 ± 4.3 ng/g
Reported Results: 3 Quantitative Results: 3
concentration (ng/g)
120
100
80
60
40
20
0
+30%
95% CI
95% CI
-30%
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

1-nitropyrene

Baltimore 2 PM

Assigned value (solid line) = 32.4 ng/g s = 5.2 ng/g 95% CL = 47.1 ng/g

Reported Results: 2 Quantitative Results: 2

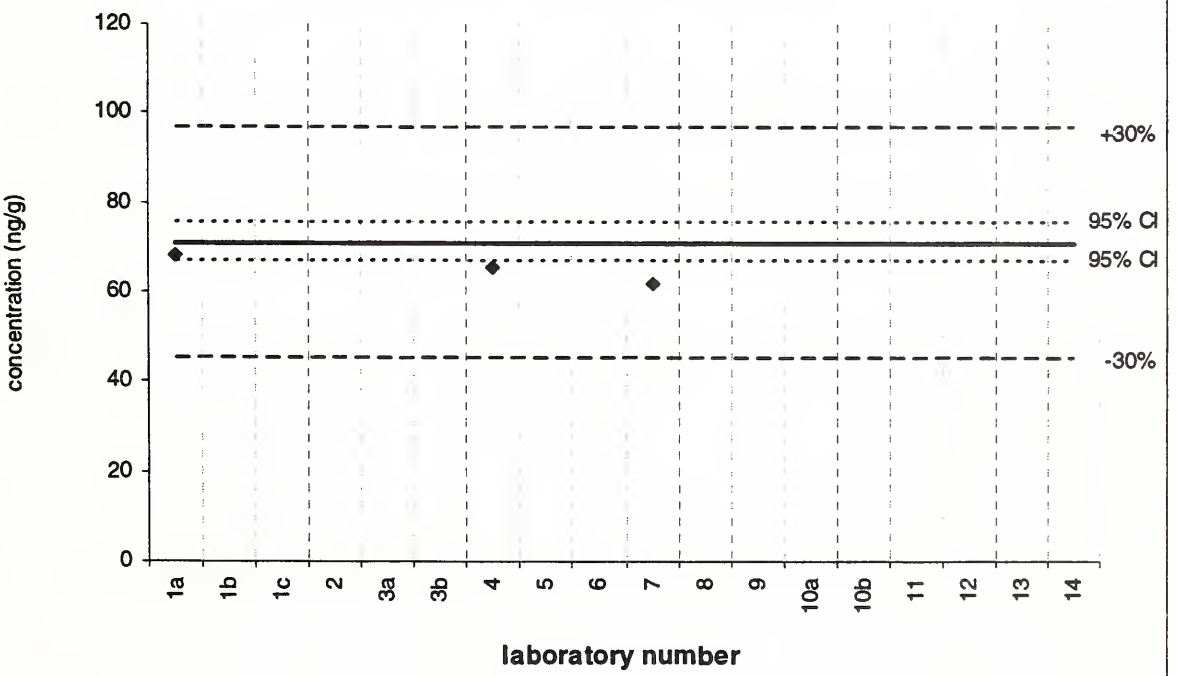


1-nitropyrene

SRM 1649a

Target Value (solid line) = 70.9 ± 4.3 ng/g

Reported Results: 3 Quantitative Results: 3

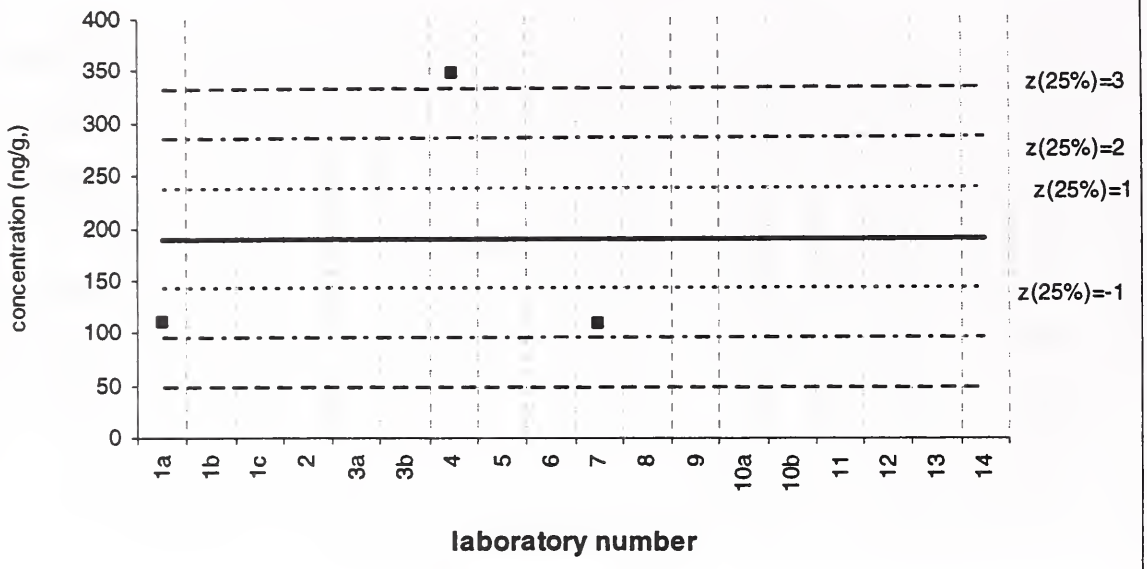


1-nitropyrene

Filter samples

Assigned value (solid line) = 189 ng/g s = 137 ng/g 95% CL = 339 ng/g

Reported Results: 3 Quantitative Results: 3

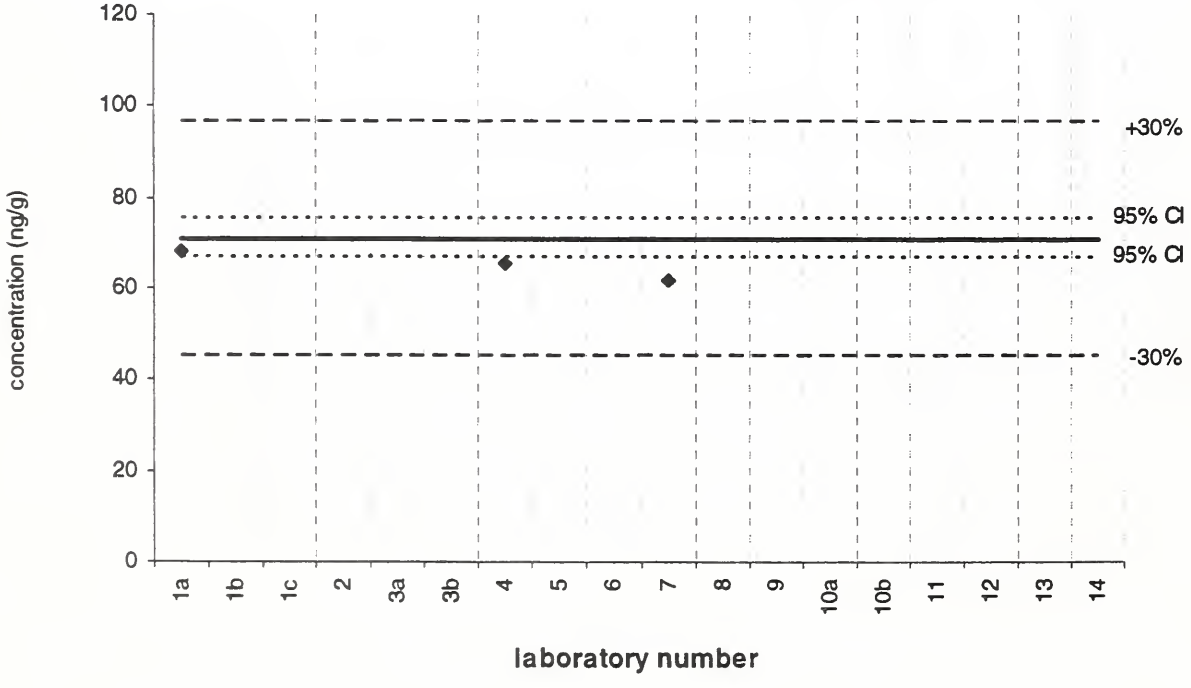


1-nitropyrene

SRM 1649a

Target Value (solid line) = 70.9 ± 4.3 ng/g

Reported Results: 3 Quantitative Results: 3

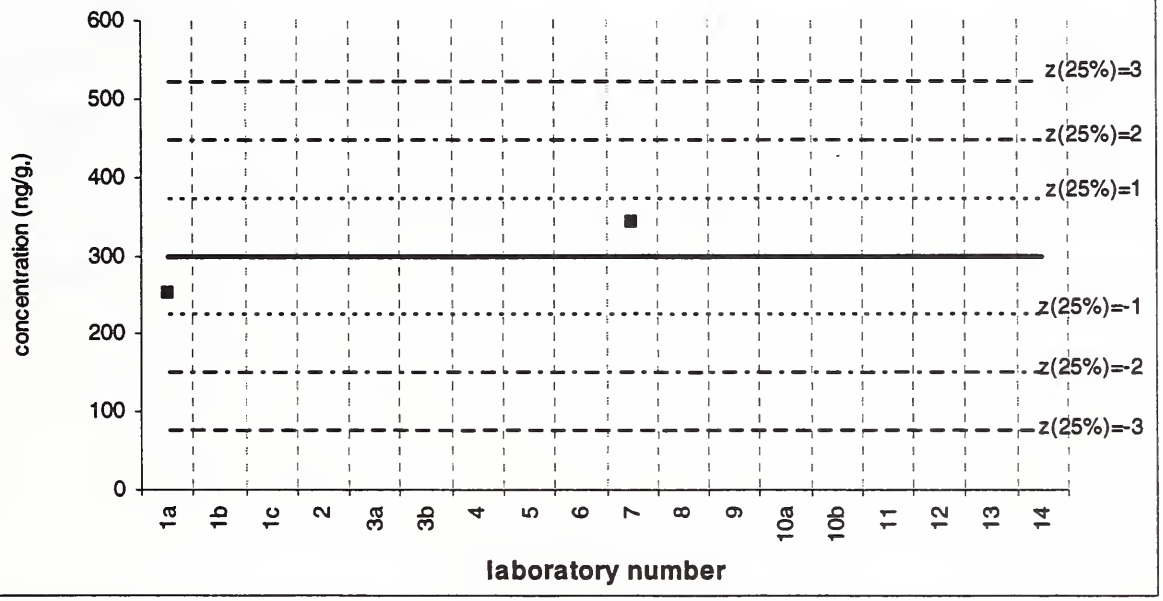


2-nitrofluoranthene

SRM 1648

Assigned value (solid line) = 297 ng/g s = 64 ng/g 95% CL = 573 ng/g

Reported Results: 2 Quantitative Results: 2

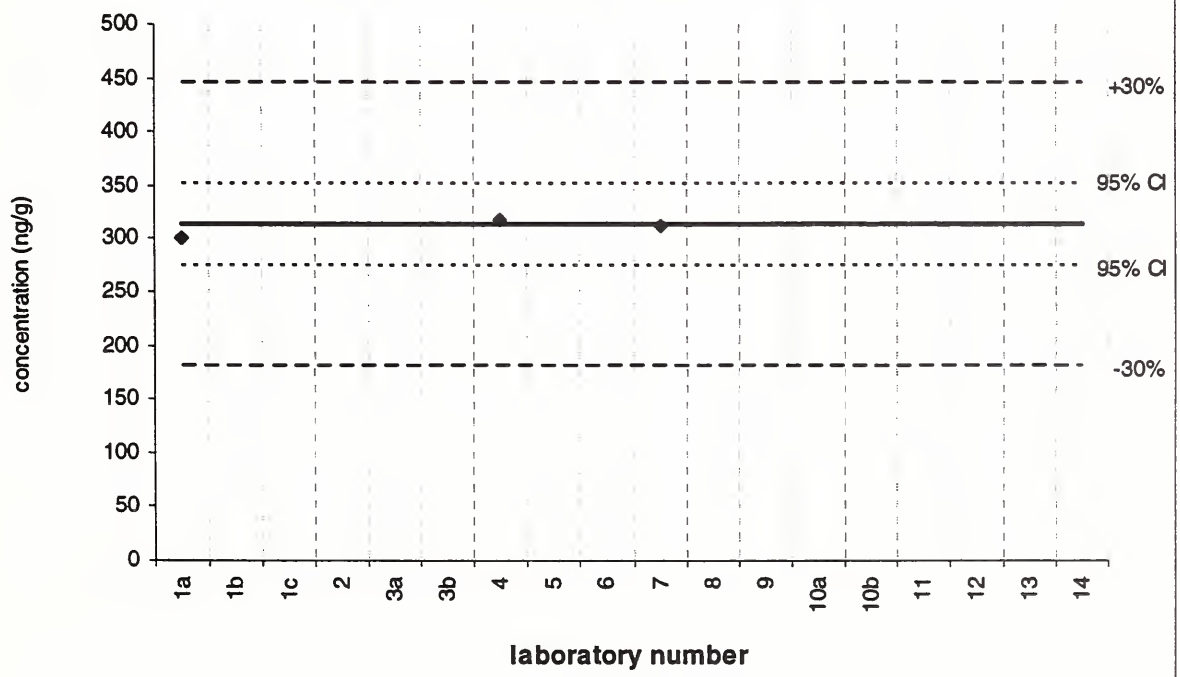


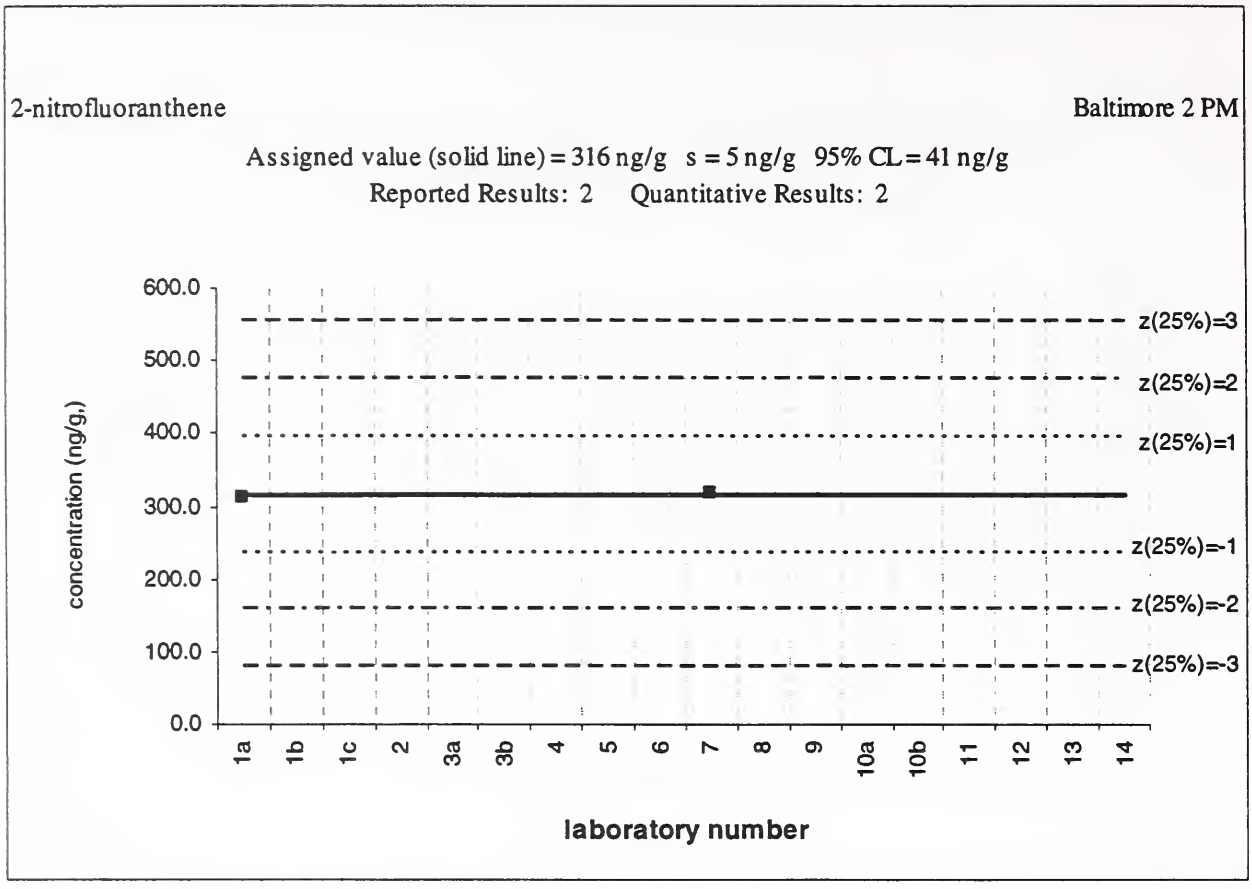
2-nitrofluoranthene

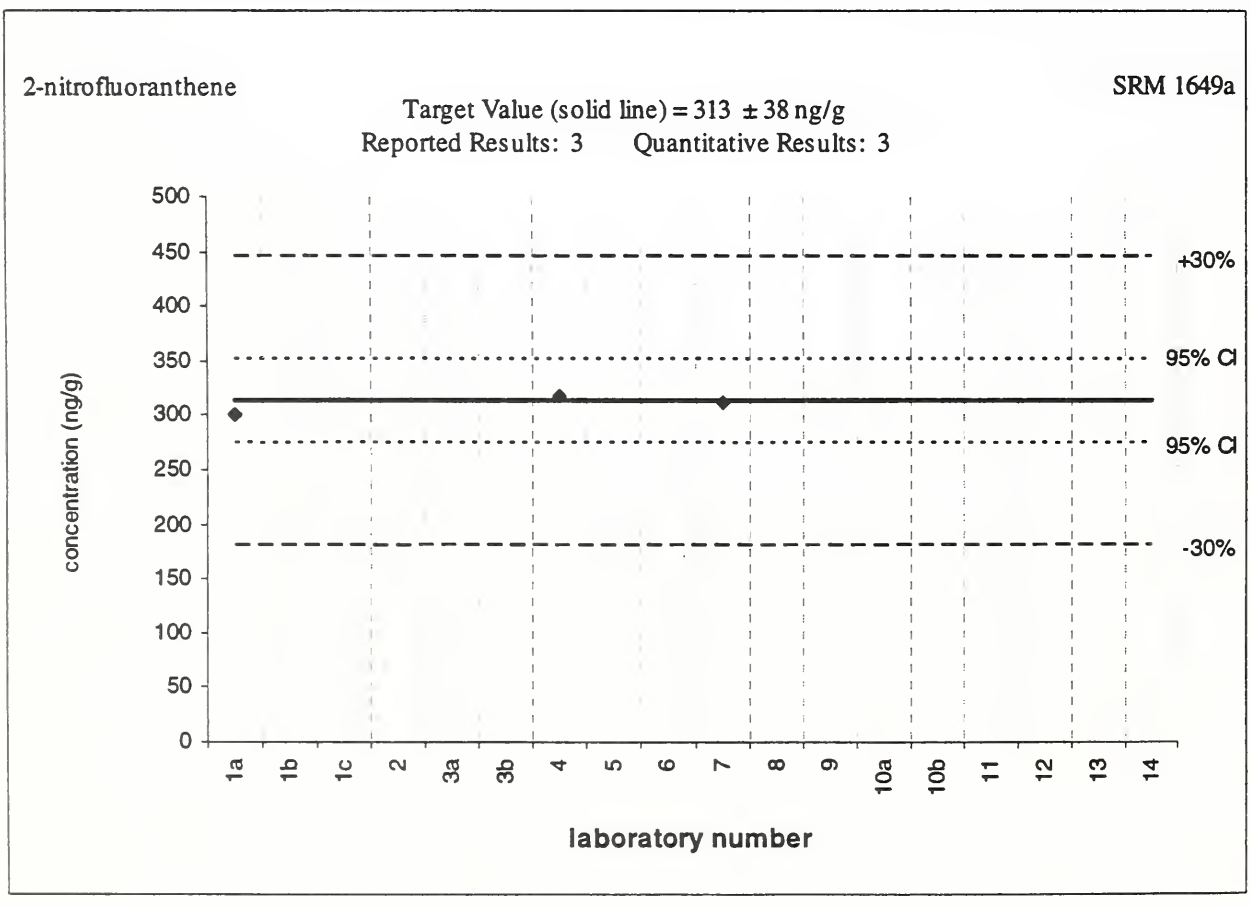
SRM 1649a

Target Value (solid line) = 313 ± 38 ng/g

Reported Results: 3 Quantitative Results: 3




2-nitrofluoranthene
Baltimore 2 PM
Assigned value (solid line) = 316 ng/g s = 5 ng/g 95% CL = 41 ng/g
Reported Results: 2 Quantitative Results: 2
600.0
500.0
400.0
300.0
200.0
100.0
0.0
concentration (ng/g.)
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

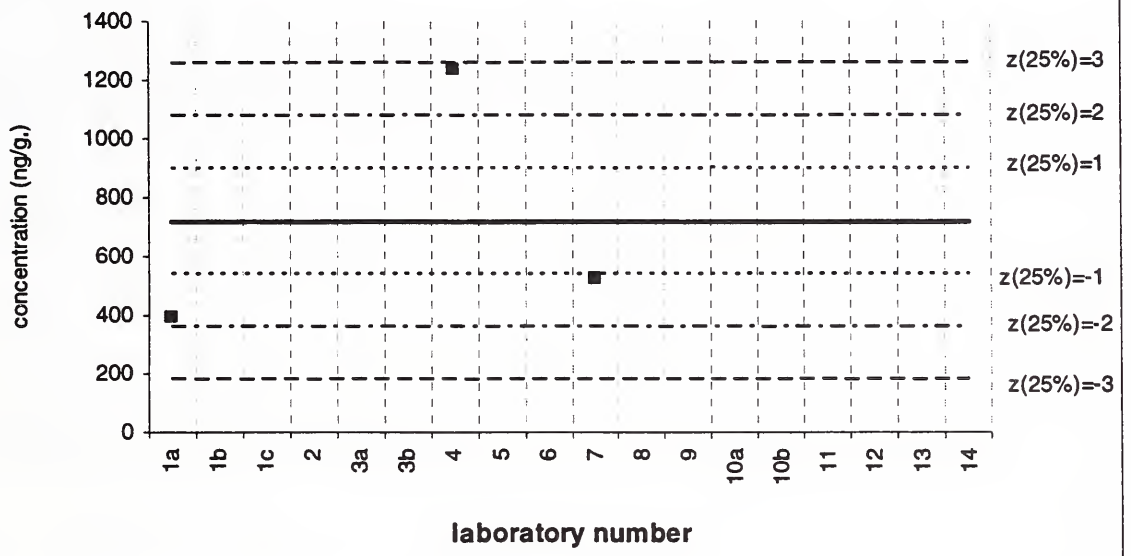

2-nitrofluoranthene
SRM 1649a
Target Value (solid line) = 313 ± 38 ng/g
Reported Results: 3 Quantitative Results: 3
500
450
400
350
300
250
200
150
100
50
0
concentration (ng/g)
+30%
95% CI
95% CI
-30%
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

2-nitrofluoranthene

Filter samples

Assigned value (solid line) = 717 ng/g s = 453 ng/g 95% CL = 1125 ng/g

Reported Results: 3 Quantitative Results: 3

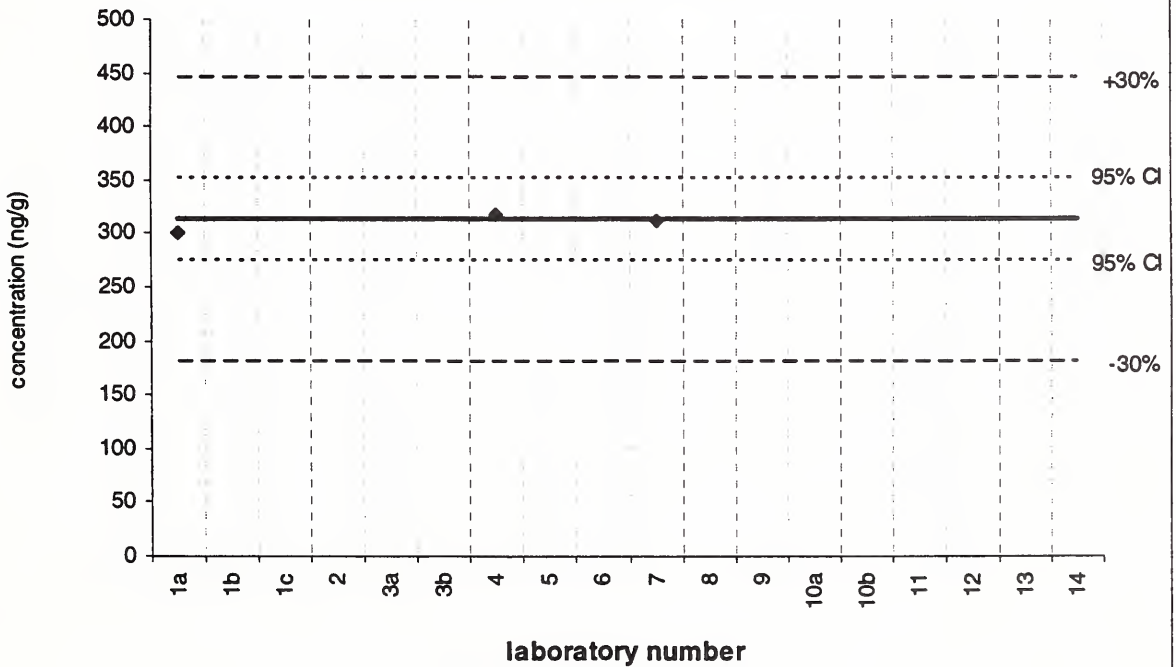


2-nitrofluoranthene

SRM 1649a

Target Value (solid line) = 313 ± 38 ng/g

Reported Results: 3 Quantitative Results: 3

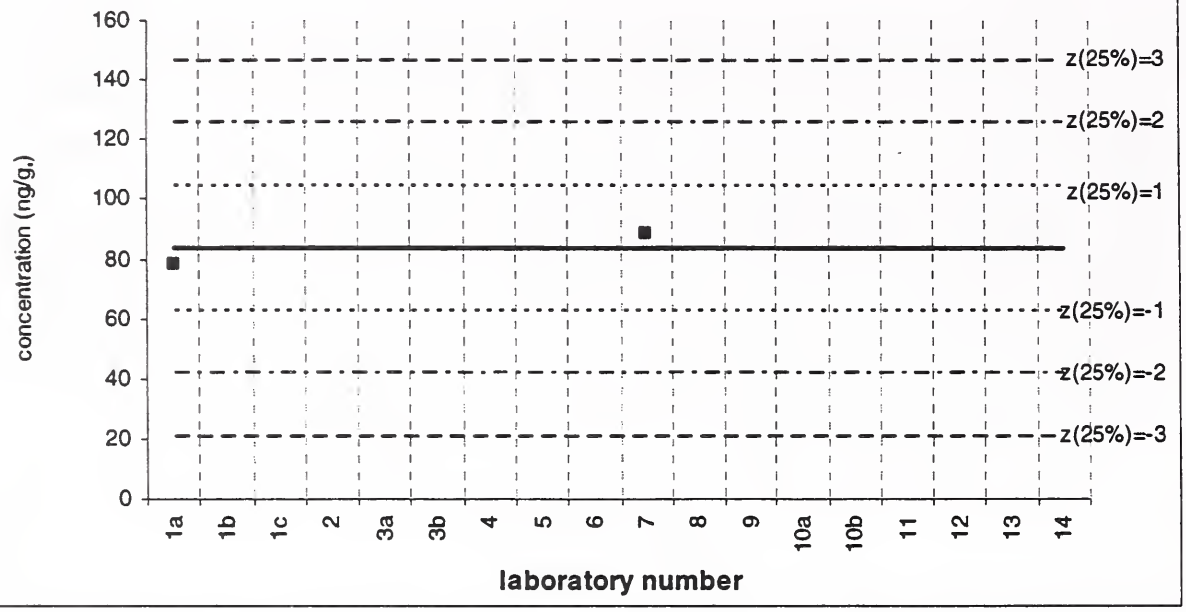


7-nitrobenz[a]anthracene

SRM 1648

Assigned value (solid line) = 83.6 ng/g s = 7.4 ng/g 95% CL = 66.6 ng/g

Reported Results: 2 Quantitative Results: 2

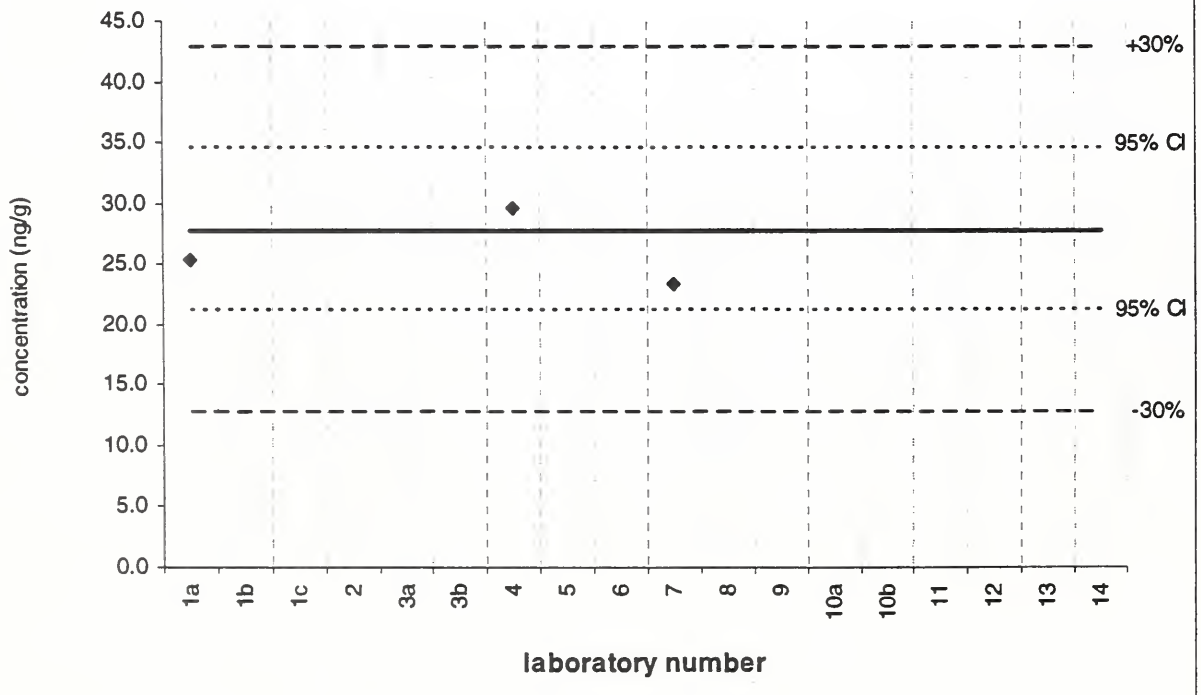


7-nitrobenz[a]anthracene

SRM 1649a

Target Value (solid line) = 27.8 ± 6.7 ng/g

Reported Results: 3 Quantitative Results: 3

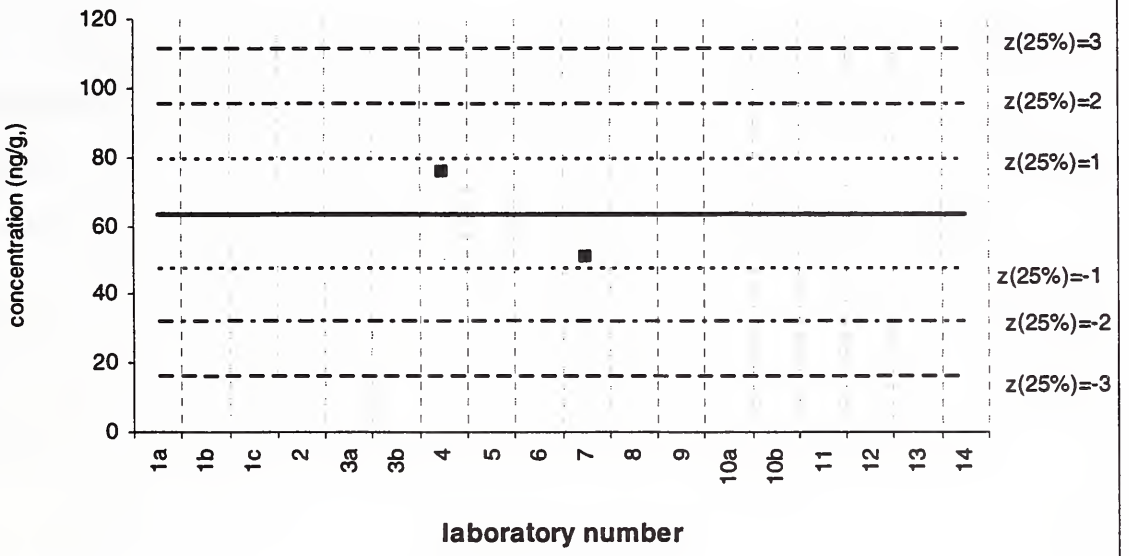


7-nitrobenz[a]anthracene

Filter samples

Assigned value (solid line) = 63.4 ng/g s = 17.7 ng/g 95% CL = 158.7 ng/g

Reported Results: 3 Quantitative Results: 2

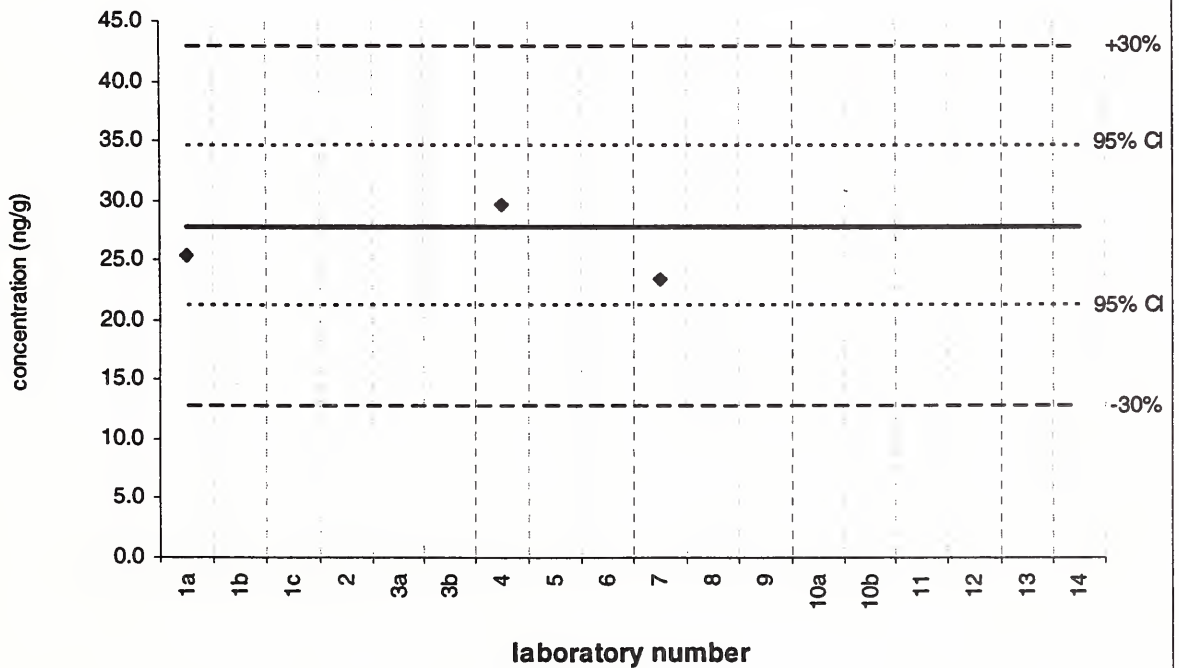


7-nitrobenz[a]anthracene

SRM 1649a

Target Value (solid line) = 27.8 ± 6.7 ng/g

Reported Results: 3 Quantitative Results: 3

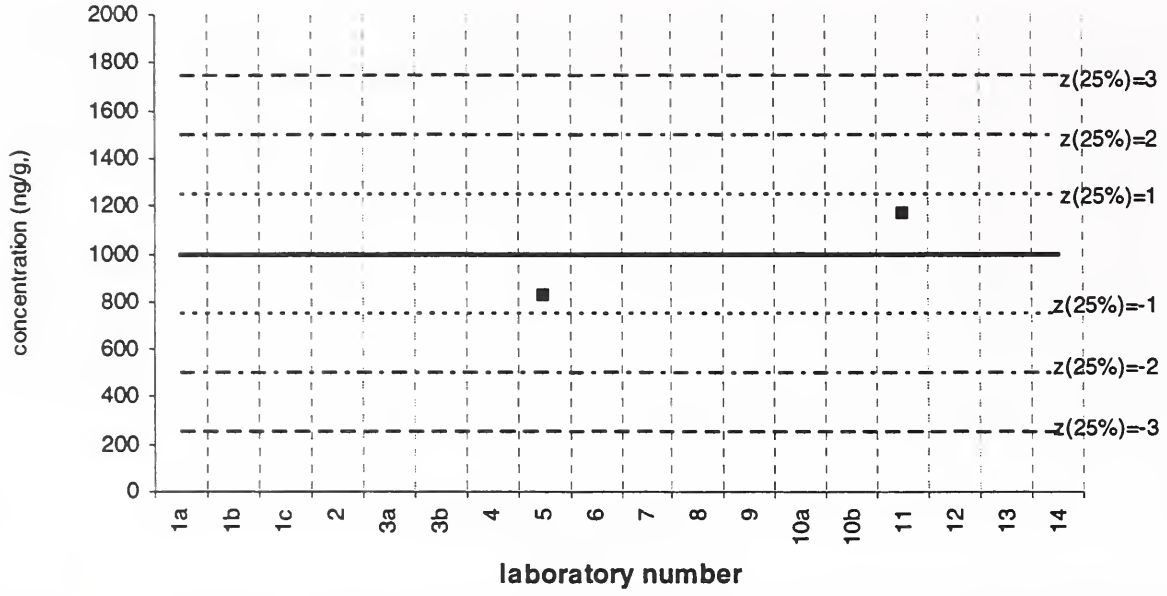


9-fluoreneone

SRM 1648

Assigned value (solid line) = 998 ng/g s = 241 ng/g 95% CL = 2168 ng/g

Reported Results: 2 Quantitative Results: 2

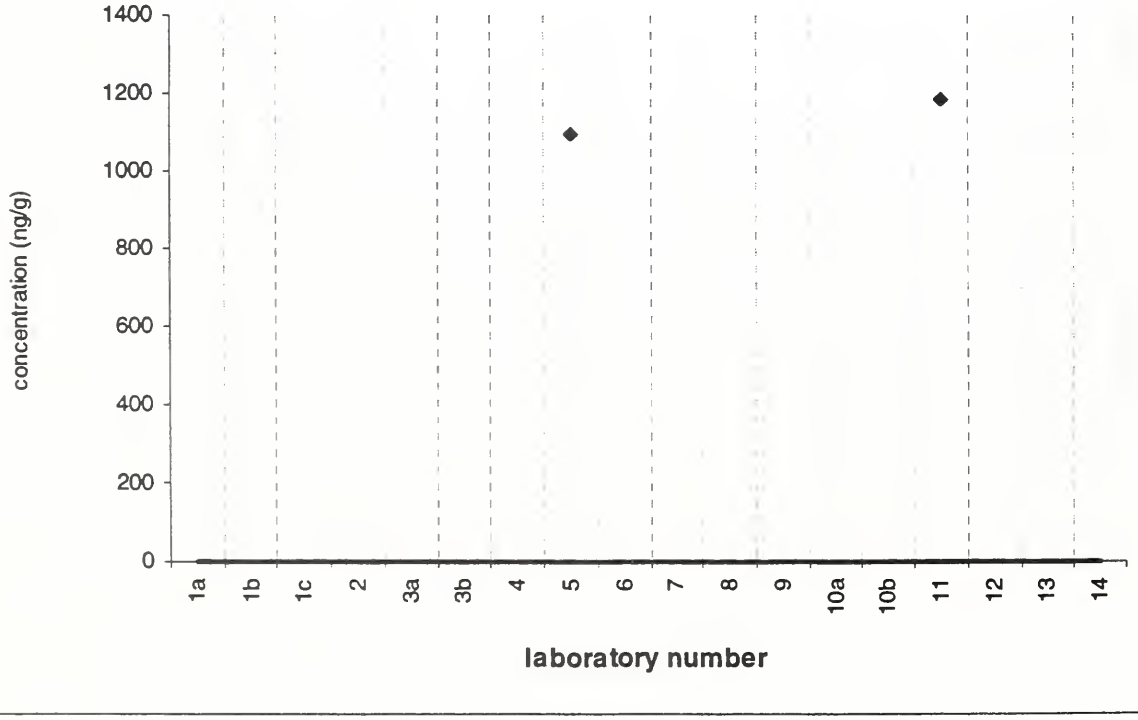


9-fluoreneone

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

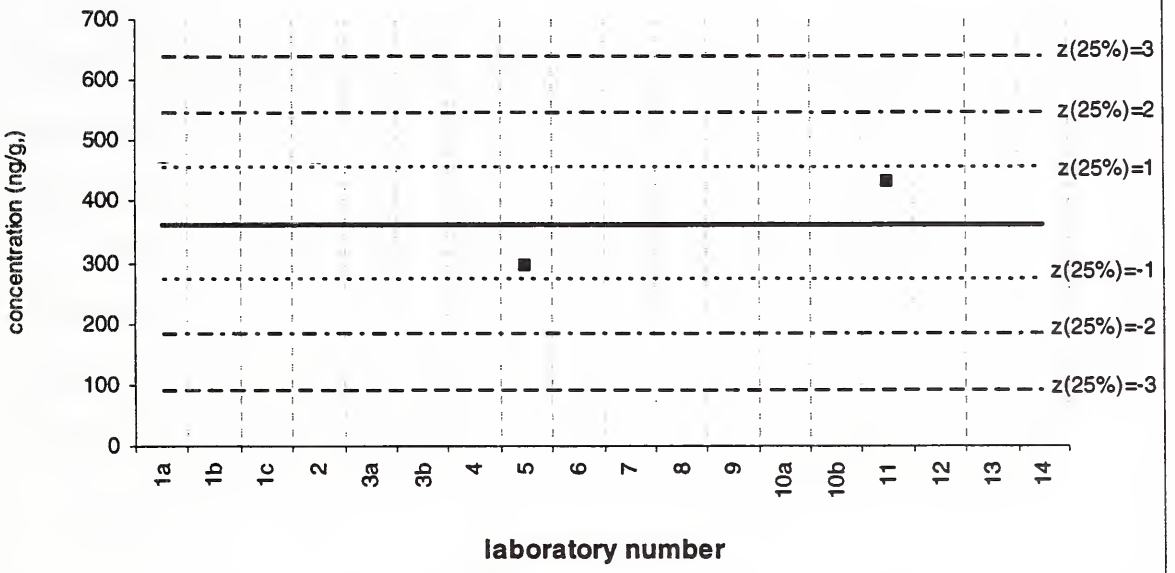


9-fluoreneone

Baltimore 2 PM

Assigned value (solid line) = 363 ng/g s = 96 ng/g 95% CL = 861 ng/g

Reported Results: 2 Quantitative Results: 2

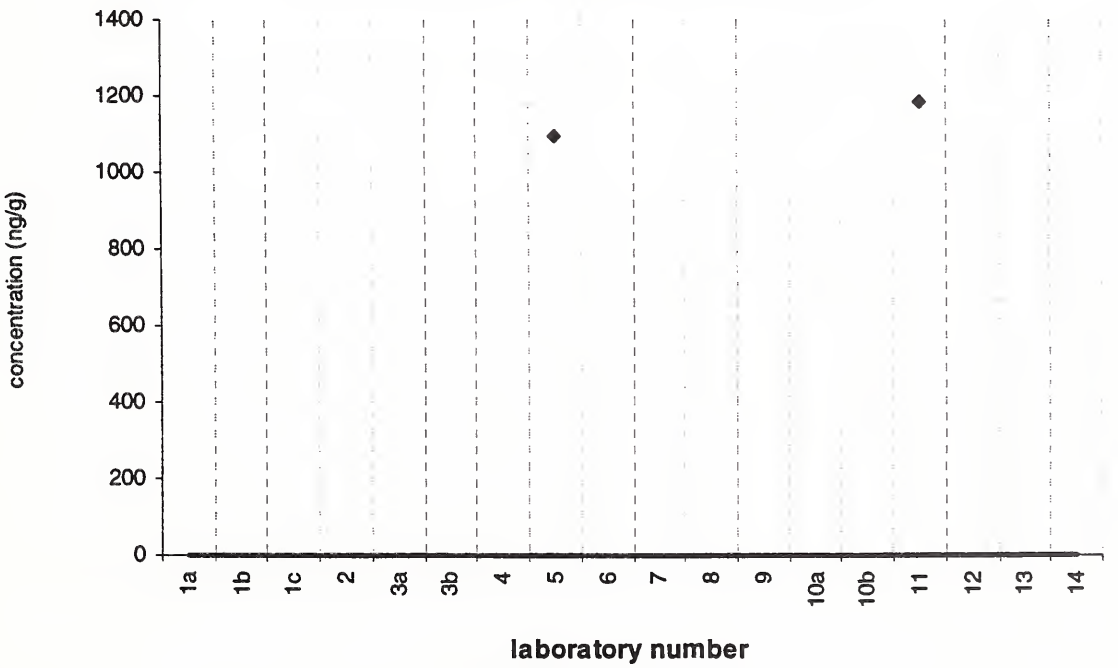


9-fluoreneone

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

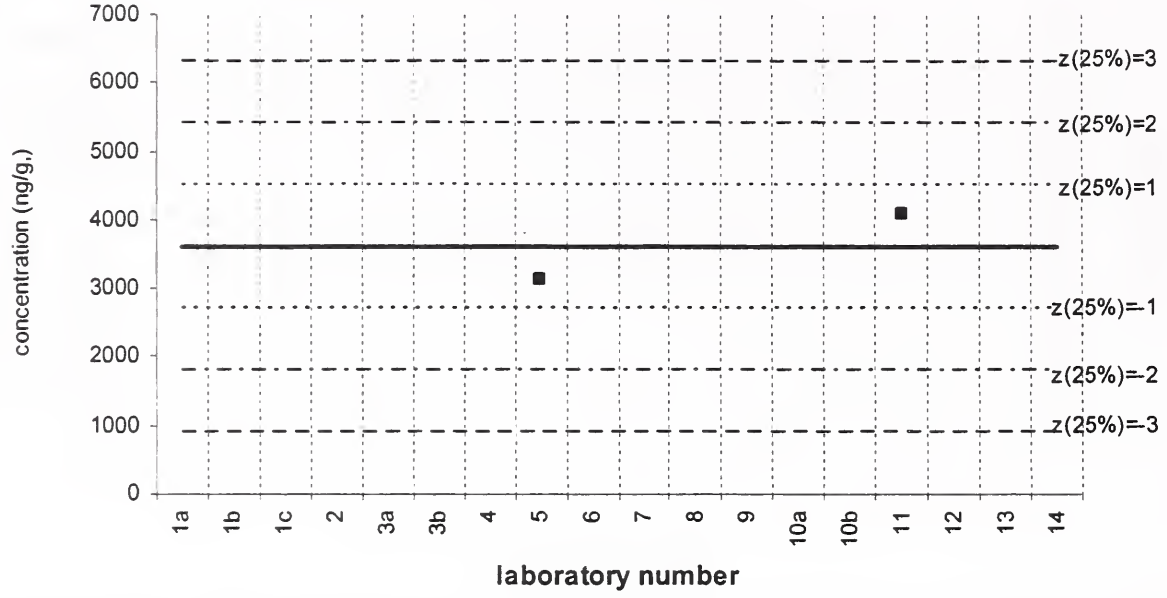


anthraquinone (9,10-AQ)

SRM 1648

Assigned value (solid line) = 3607 ng/g s = 697 ng/g 95% CL = 6261 ng/g

Reported Results: 2 Quantitative Results: 2

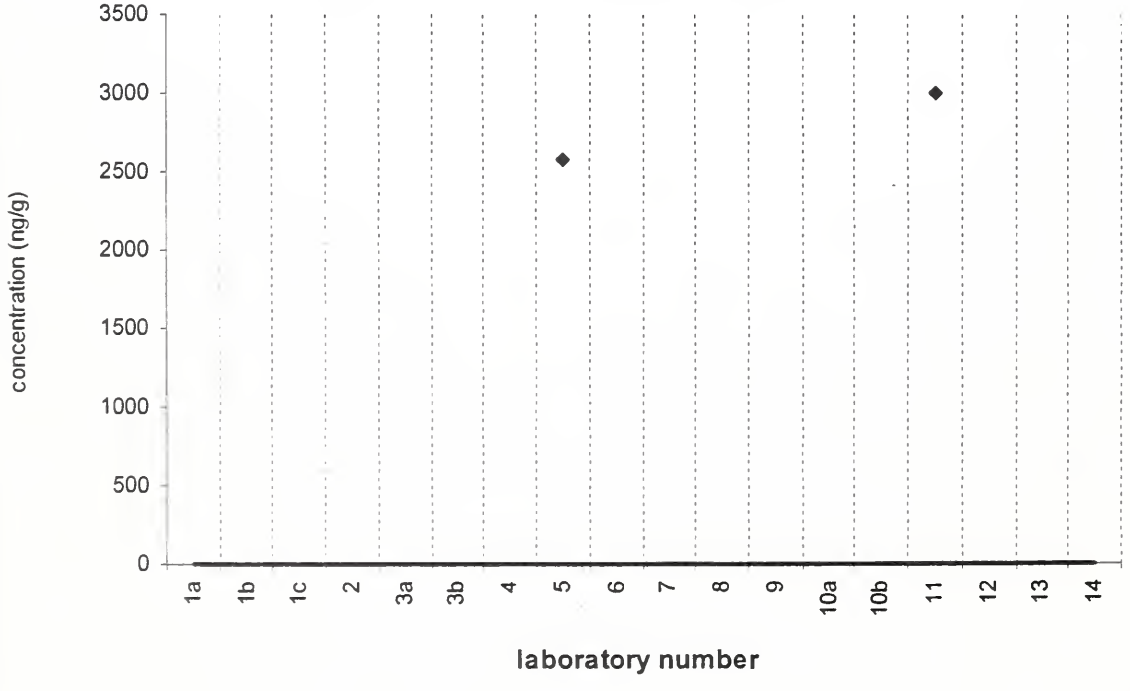


anthraquinone (9,10-AQ)

SRM 1649a

Target Value = no target ng/g

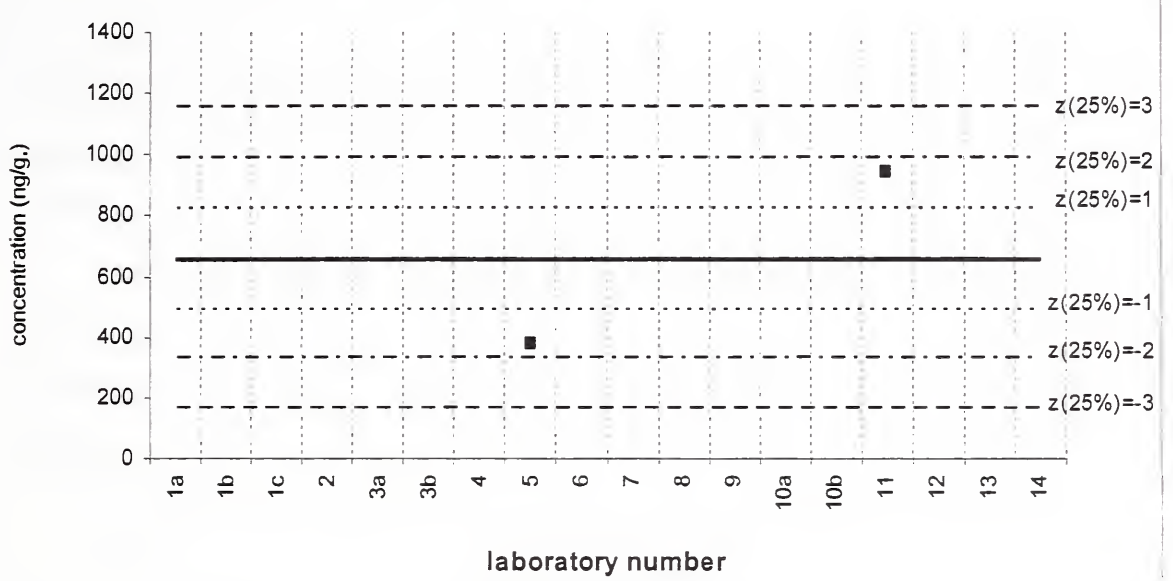
Reported Results: 2 Quantitative Results: 2



anthraquinone (9,10-AQ) Baltimore 2 PM

Assigned value (solid line) = 658 ng/g s = 399 ng/g 95% CL = 3582 ng/g

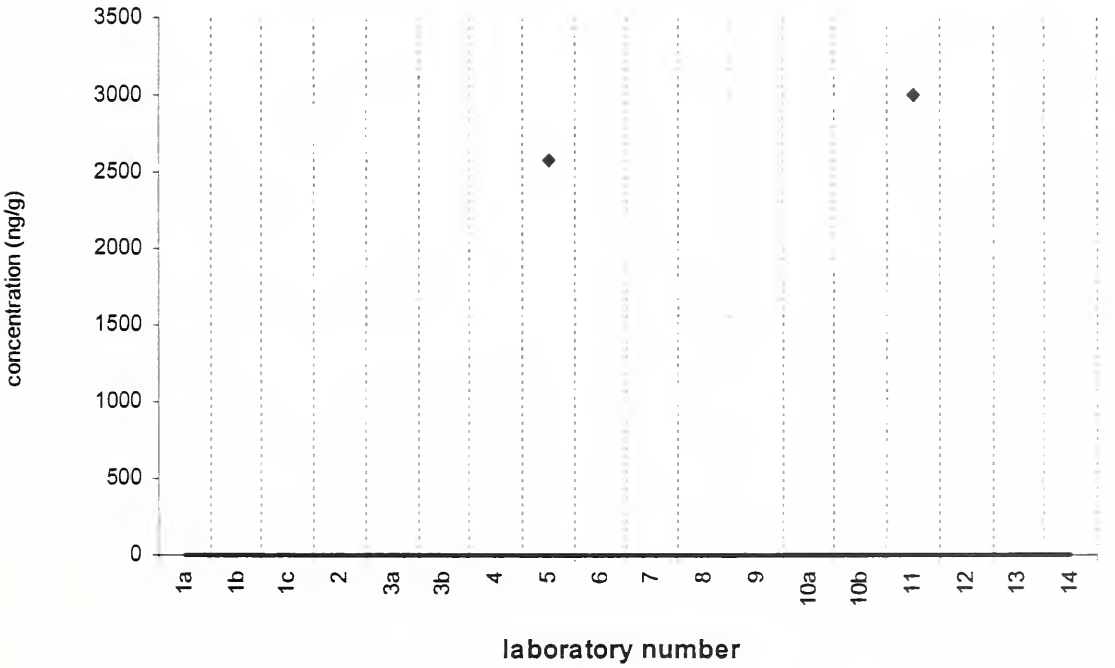
Reported Results: 2 Quantitative Results: 2



anthraquinone (9,10-AQ) SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

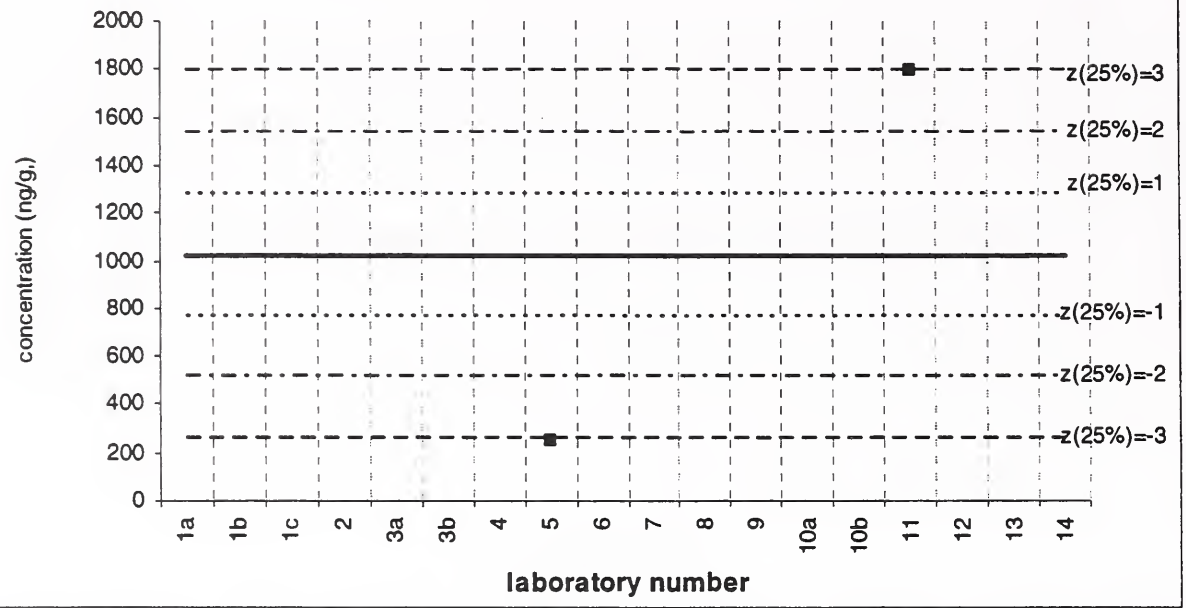


benzanthrone

SRM 1648

Assigned value (solid line) = 1024 ng/g s = 1091 ng/g 95% CL = 9806 ng/g

Reported Results: 2 Quantitative Results: 2

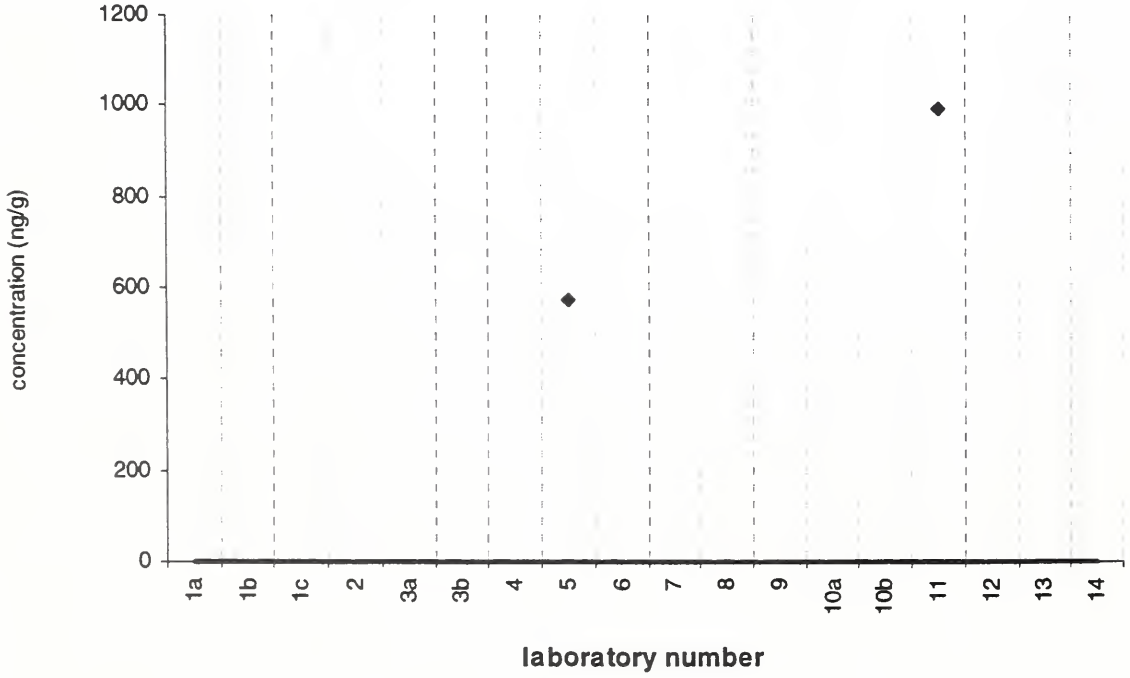


benzanthrone

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

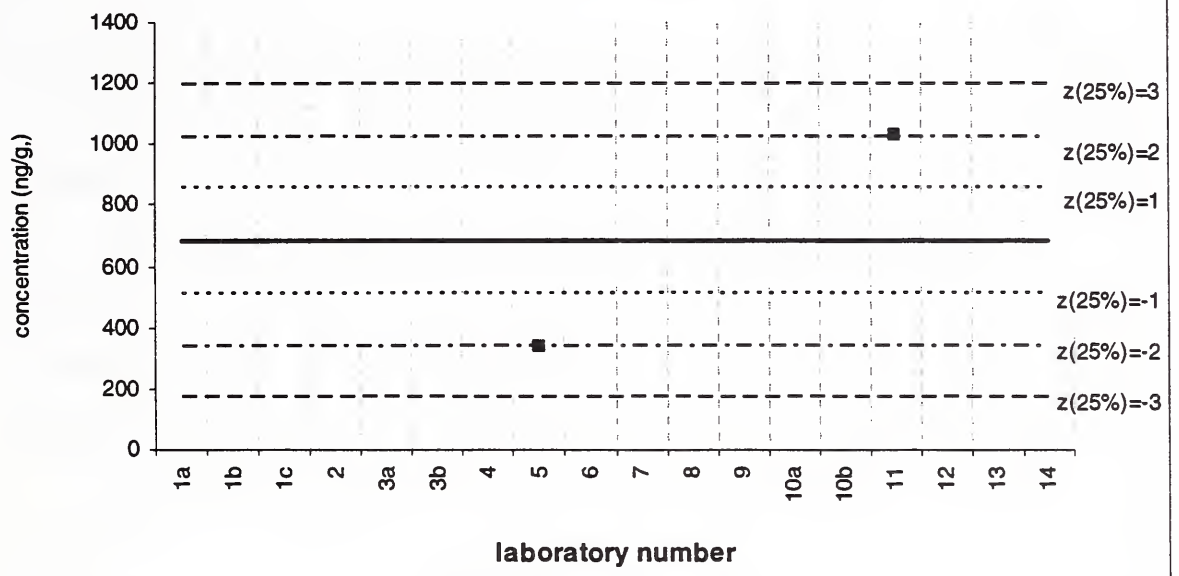


benzanthrone

Baltimore 2 PM

Assigned value (solid line) = 682 ng/g s = 486 ng/g 95% CL = 4366 ng/g

Reported Results: 2 Quantitative Results: 2

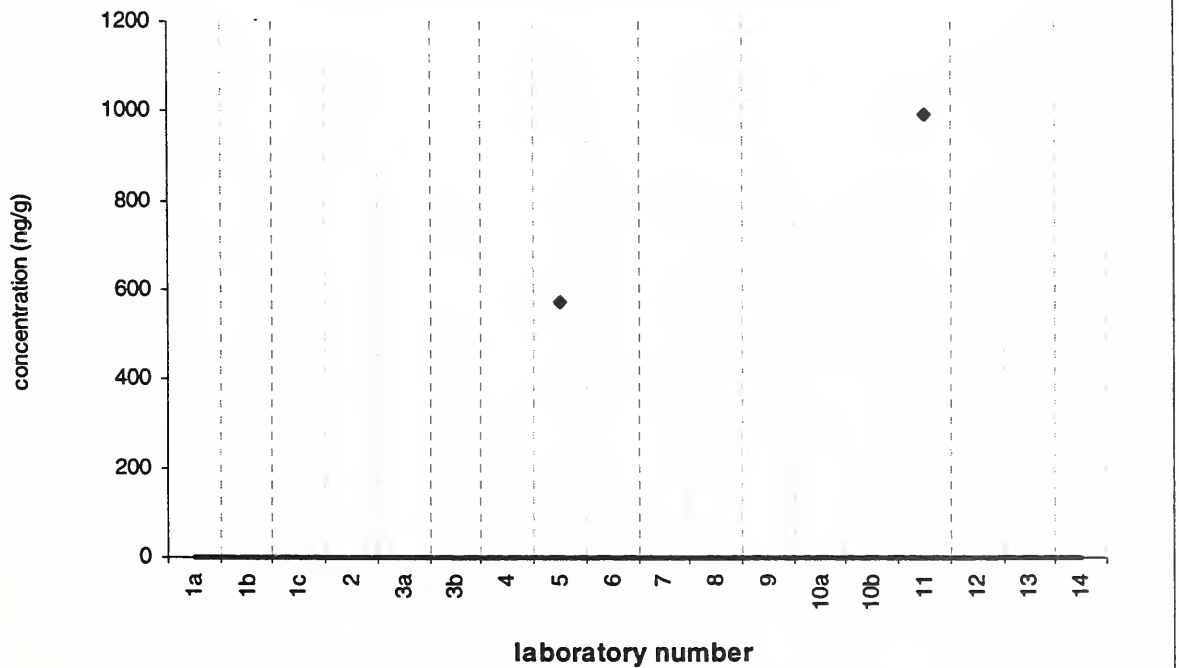


benzanthrone

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

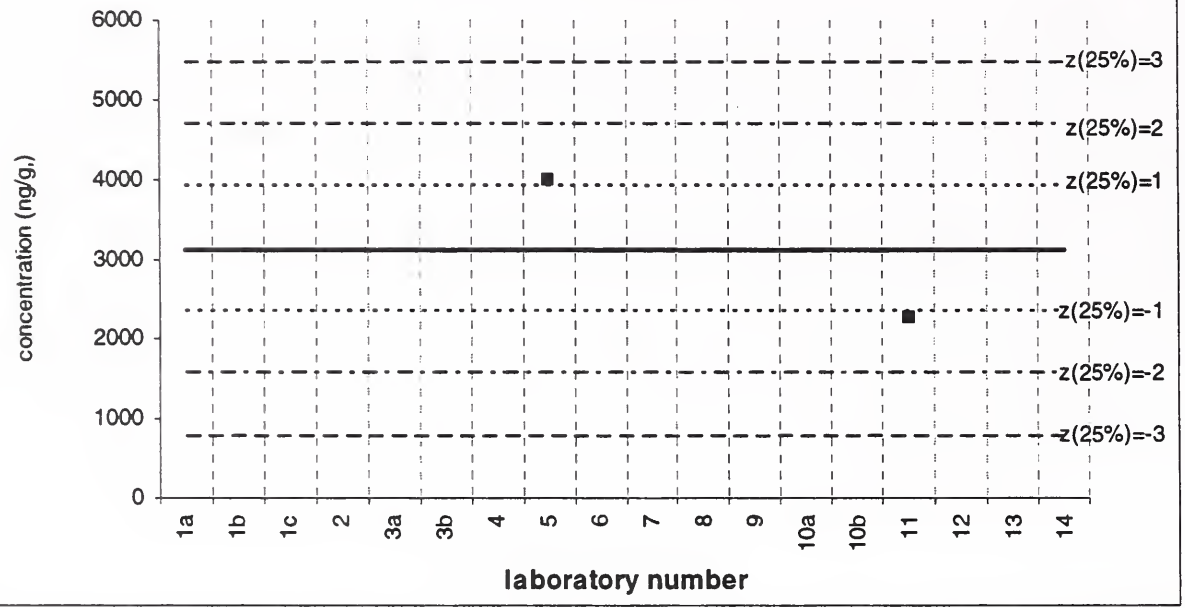


benz[a]anthracene-7,12-dione

SRM 1648

Assigned value (solid line) = 3121 ng/g s = 1225 ng/g 95% CL = 11004 ng/g

Reported Results: 2 Quantitative Results: 2

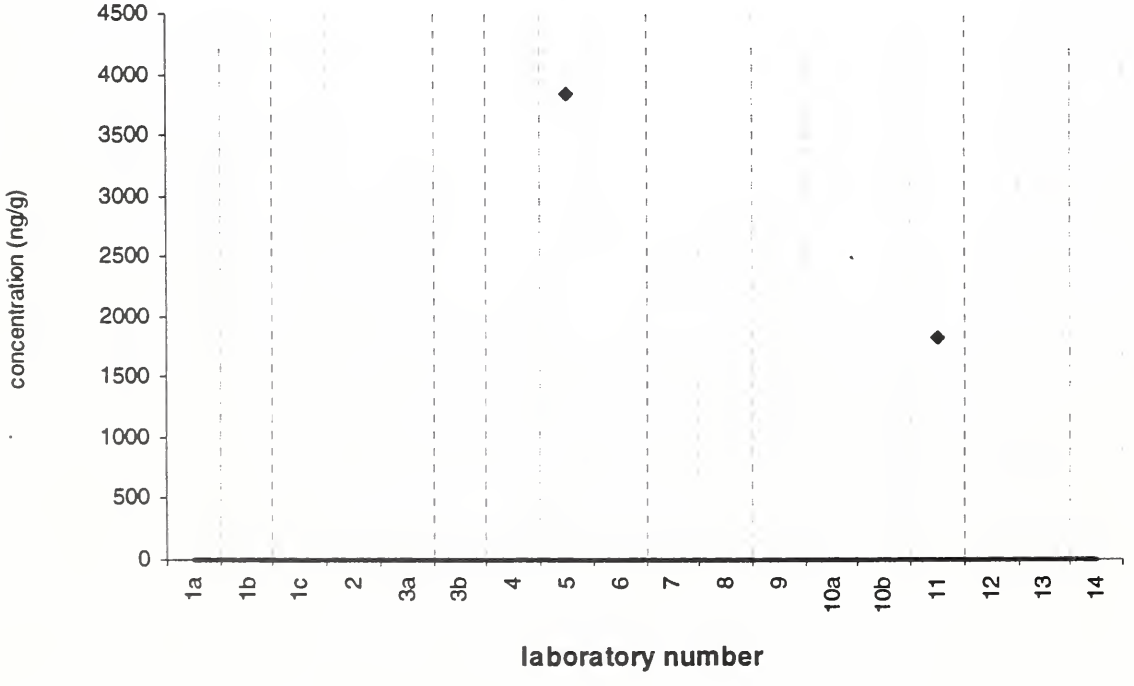


benz[a]anthracene-7,12-dione

SRM 1649a

Target Value = no target ng/g

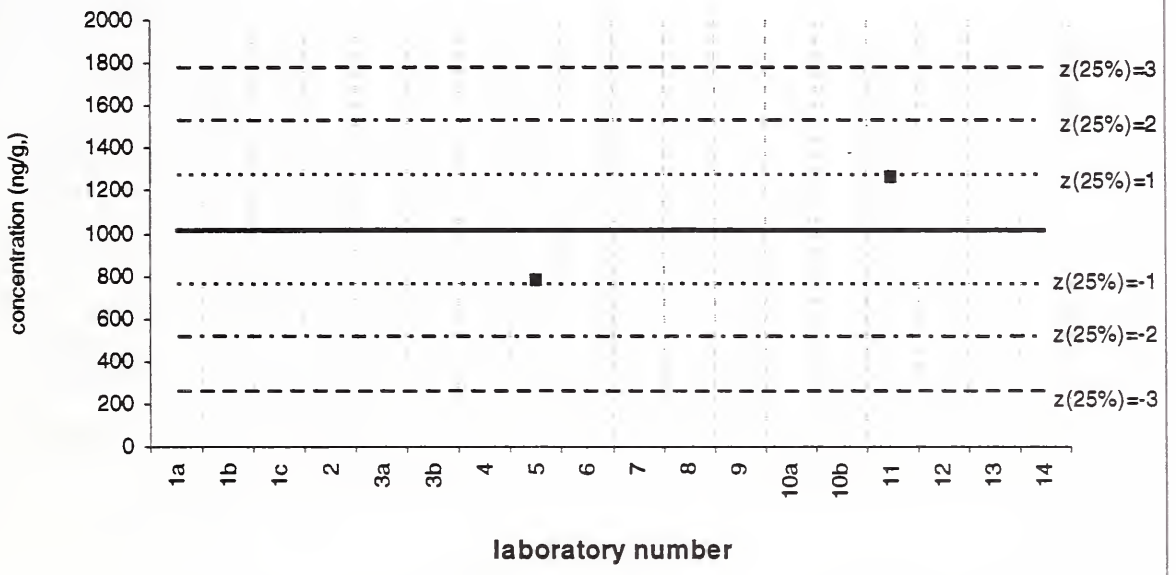
Reported Results: 2 Quantitative Results: 2



benz[a]anthracene-7,12-dione Baltimore 2 PM

Assigned value (solid line) = 1015 ng/g s = 342 ng/g 95% CL = 3069 ng/g

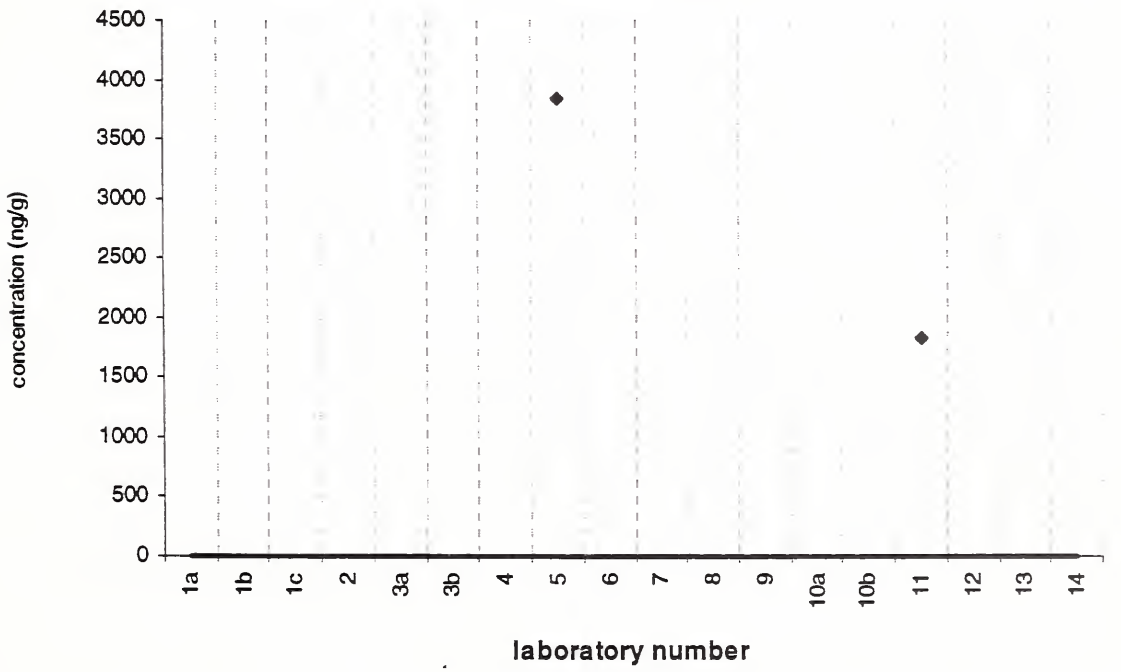
Reported Results: 2 Quantitative Results: 2

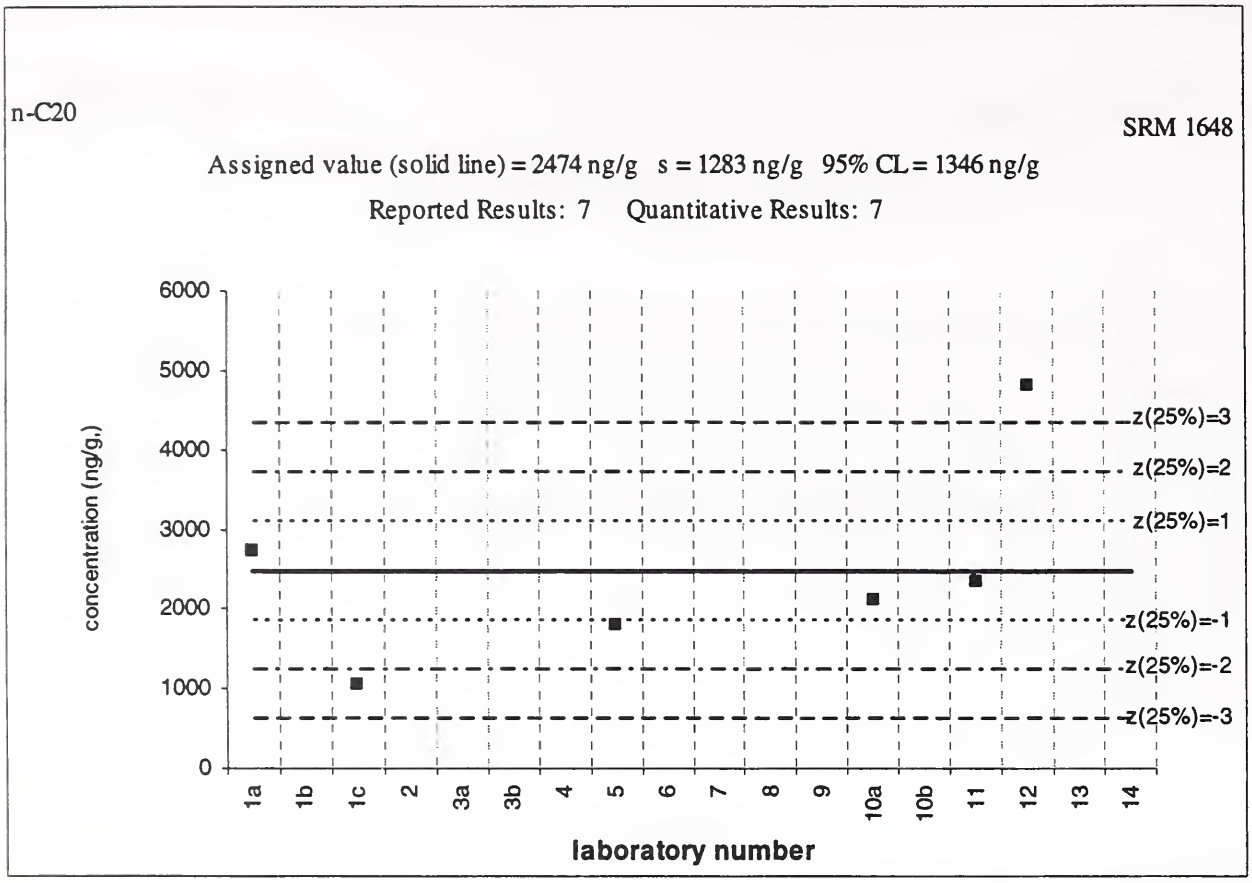


benz[a]anthracene-7,12-dione SRM 1649a

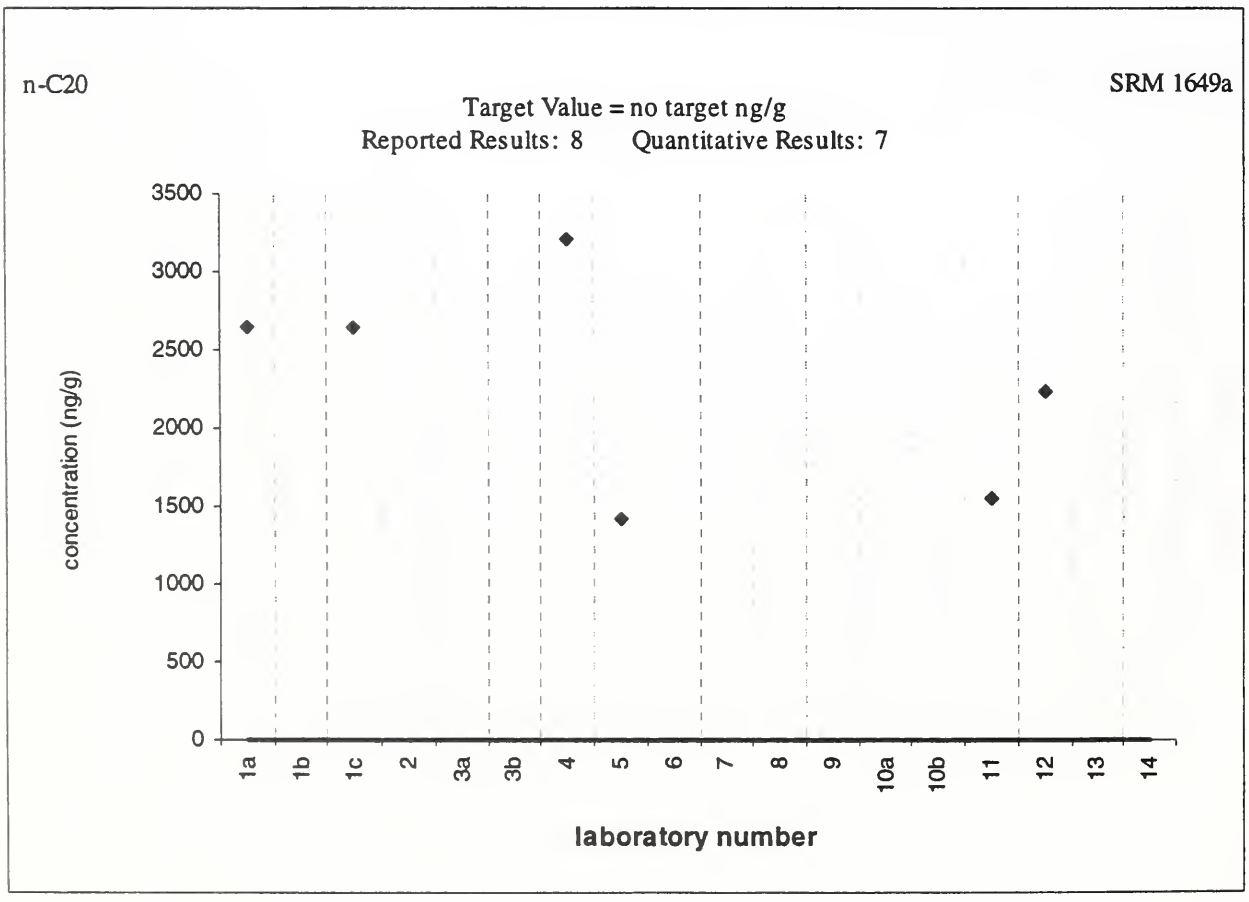
Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

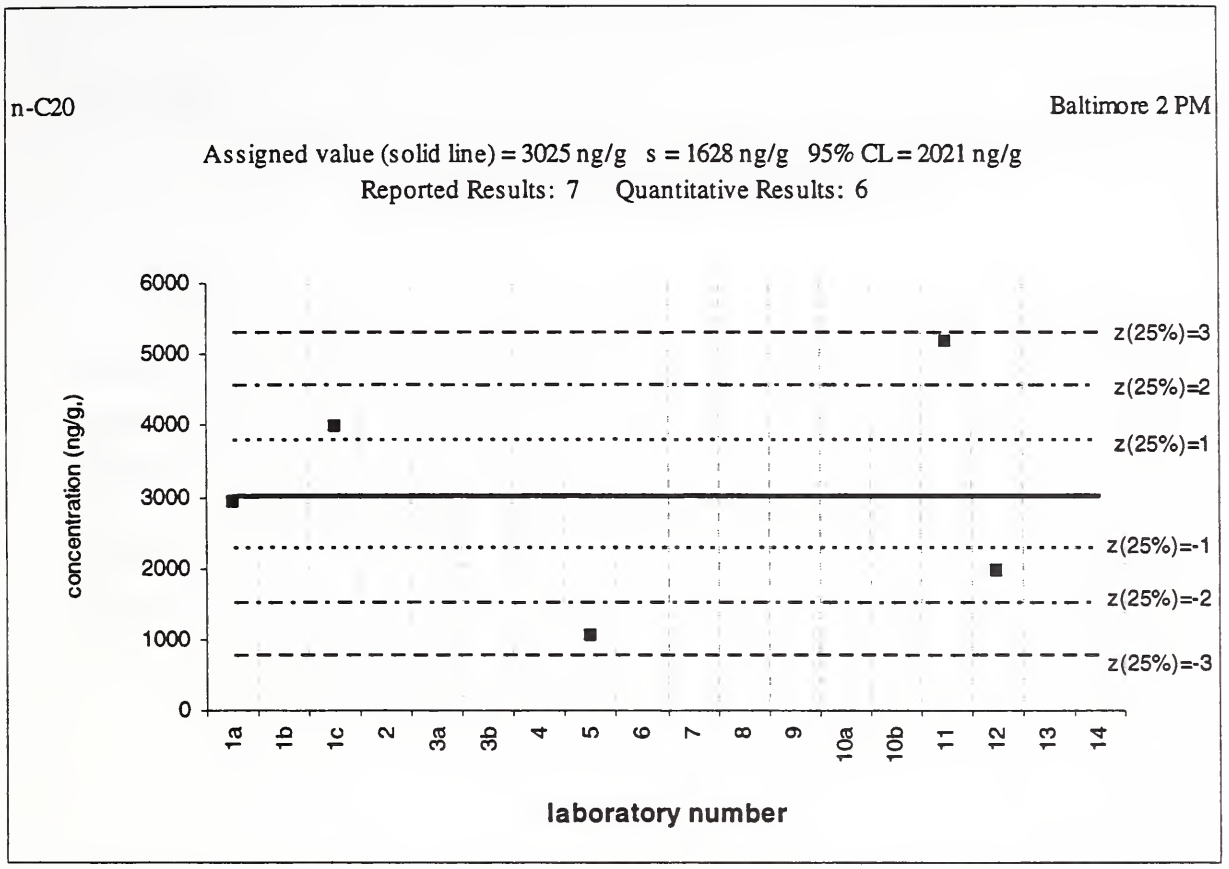




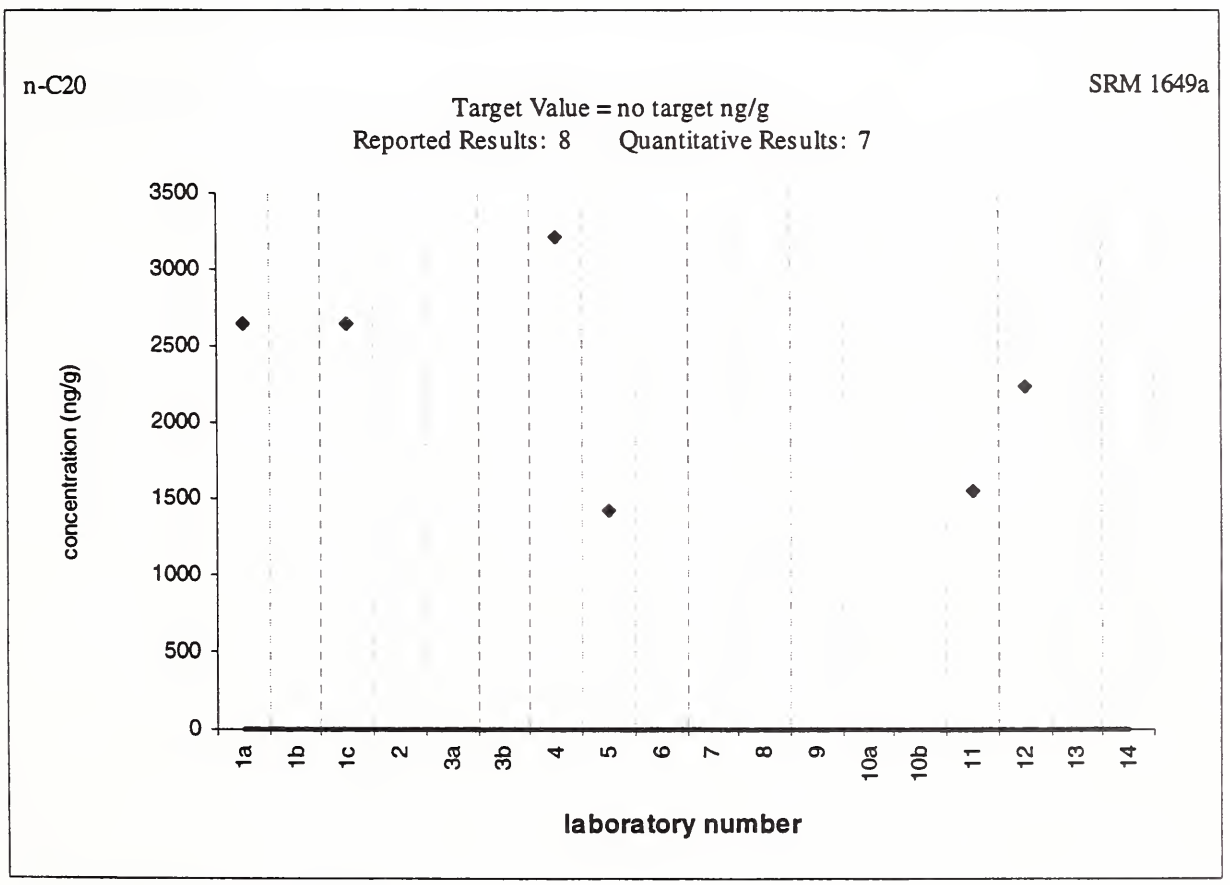
lab 9 = 19546 ng/g



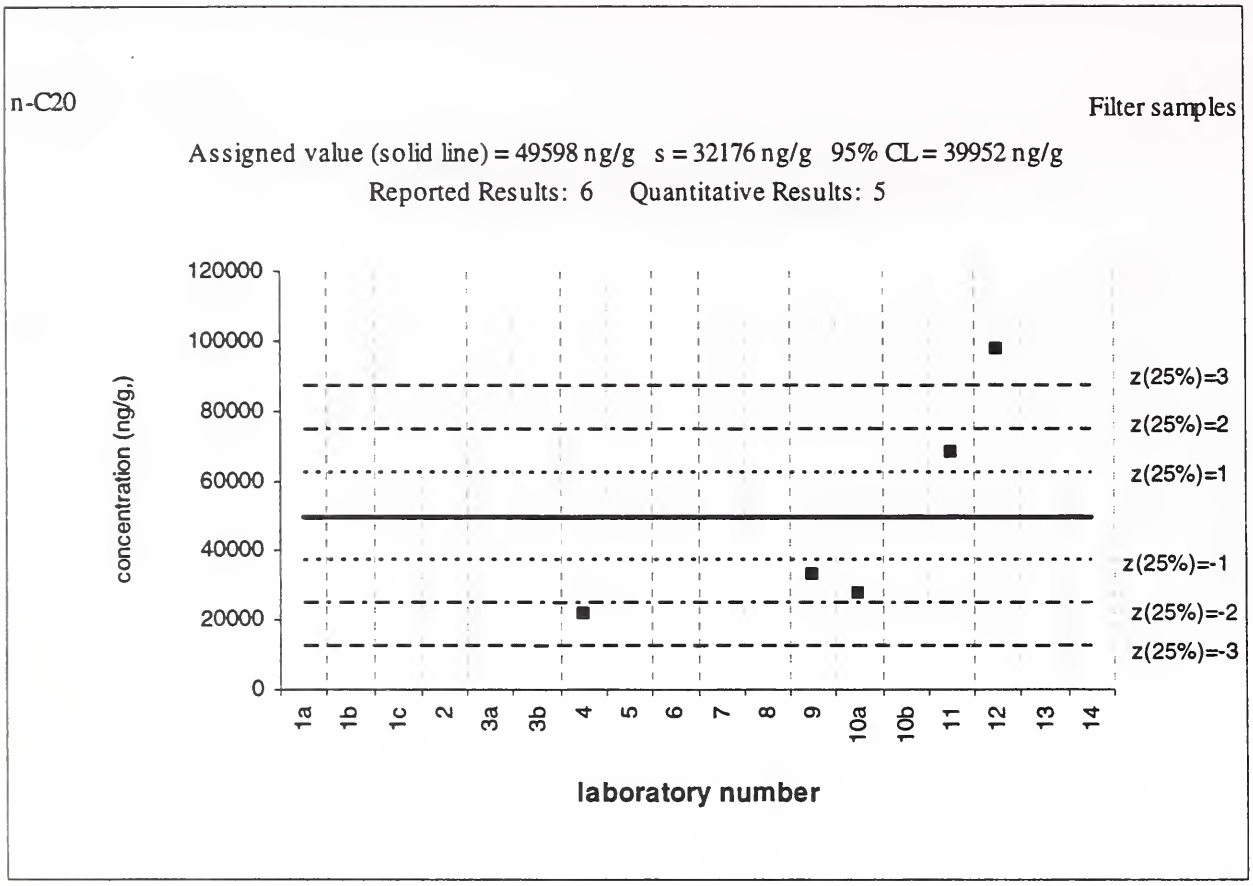
lab 9 = 18662 ng/g

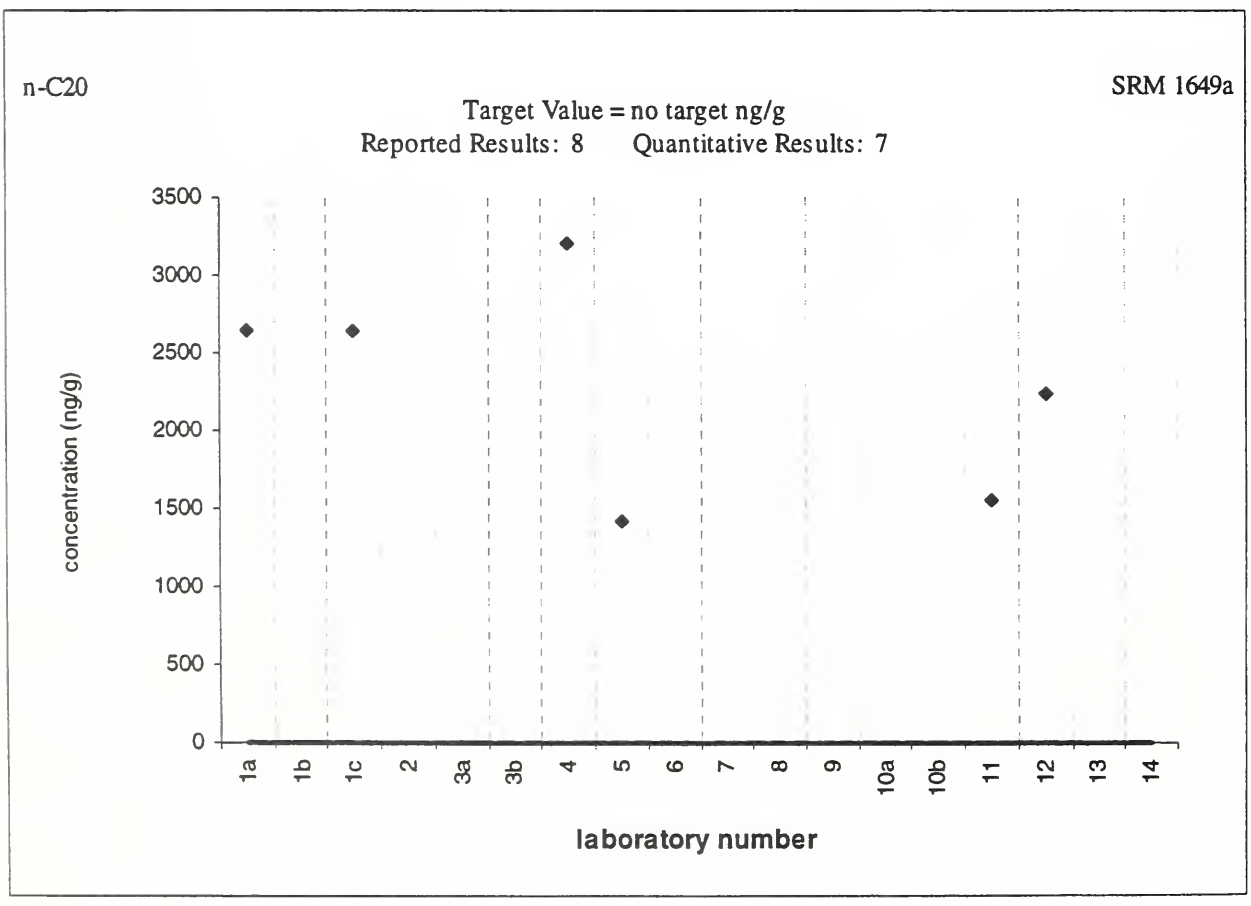


lab 9 = 32807 ng/g



lab 9 = 18662 ng/g





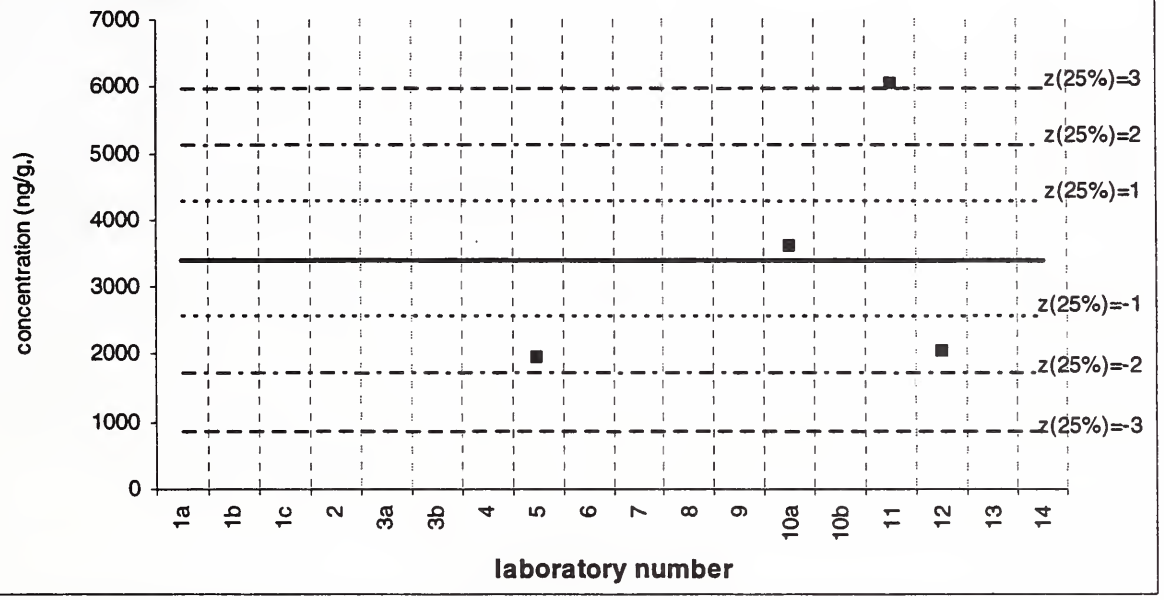
lab 9 = 18662 ng/g

n-C21

SRM 1648

Assigned value (solid line) = 3406 ng/g s = 1915 ng/g 95% CL = 3047 ng/g

Reported Results: 4 Quantitative Results: 4

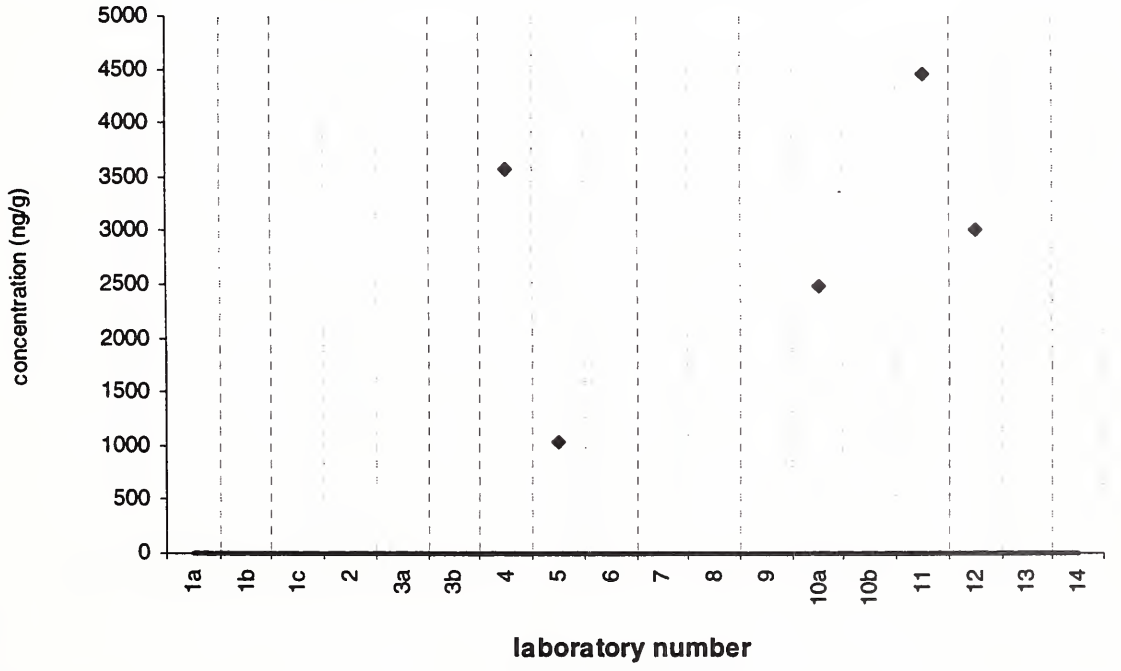


n-C21

SRM 1649a

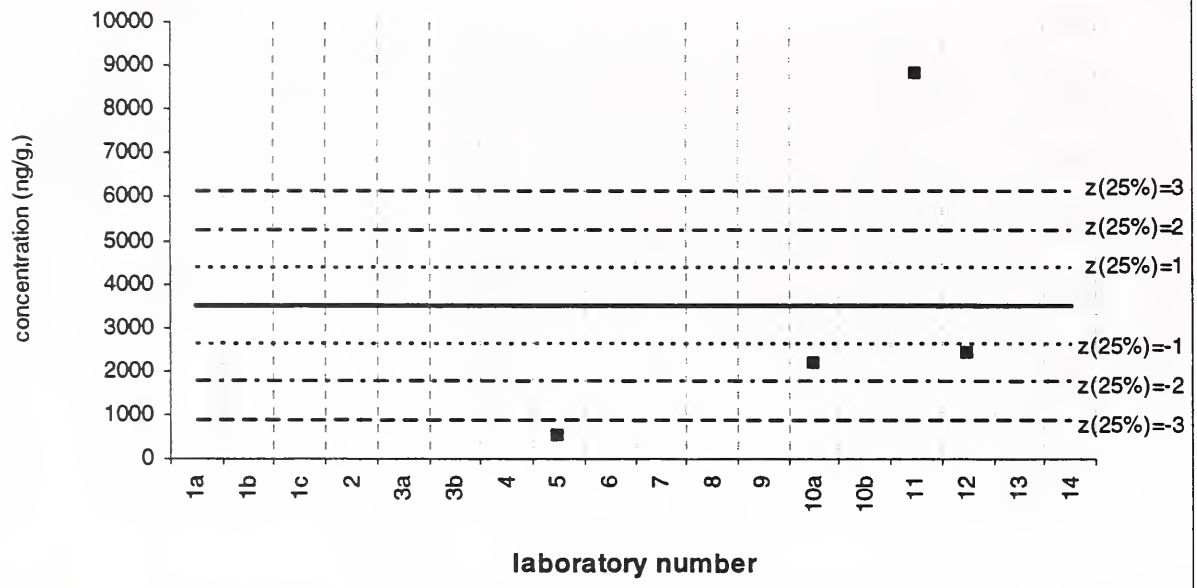
Target Value = no target ng/g

Reported Results: 5 Quantitative Results: 5



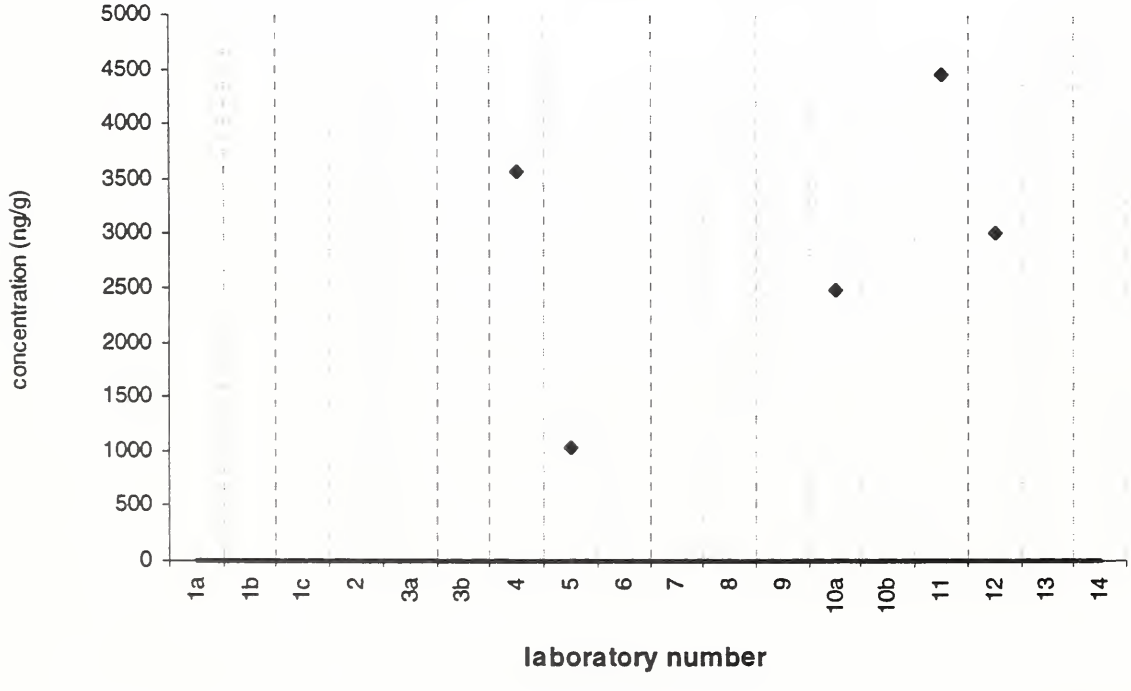
n-C21 Baltimore 2 PM

Assigned value (solid line) = 3488 ng/g s = 3655 ng/g 95% CL = 5817 ng/g
Reported Results: 4 Quantitative Results: 4



n-C21 SRM 1649a

Target Value = no target ng/g
Reported Results: 5 Quantitative Results: 5



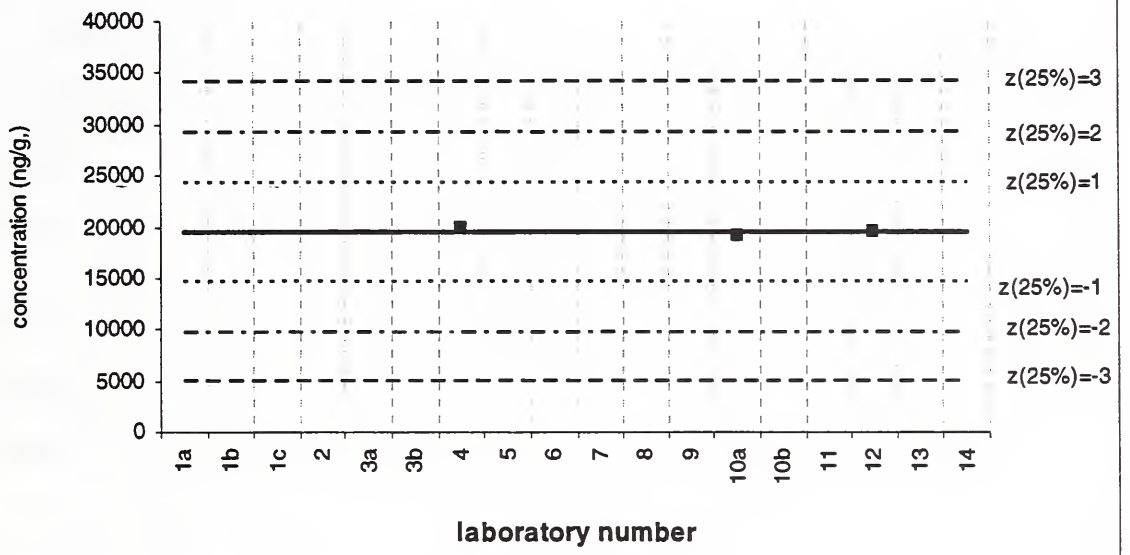
n-C21

Filter samples

Assigned value (solid line) = 19458 ng/g s = 446 ng/g 95% CL = 1109 ng/g

Reported Results: 4 Quantitative Results: 4

lab 11 = 215302 ng/g

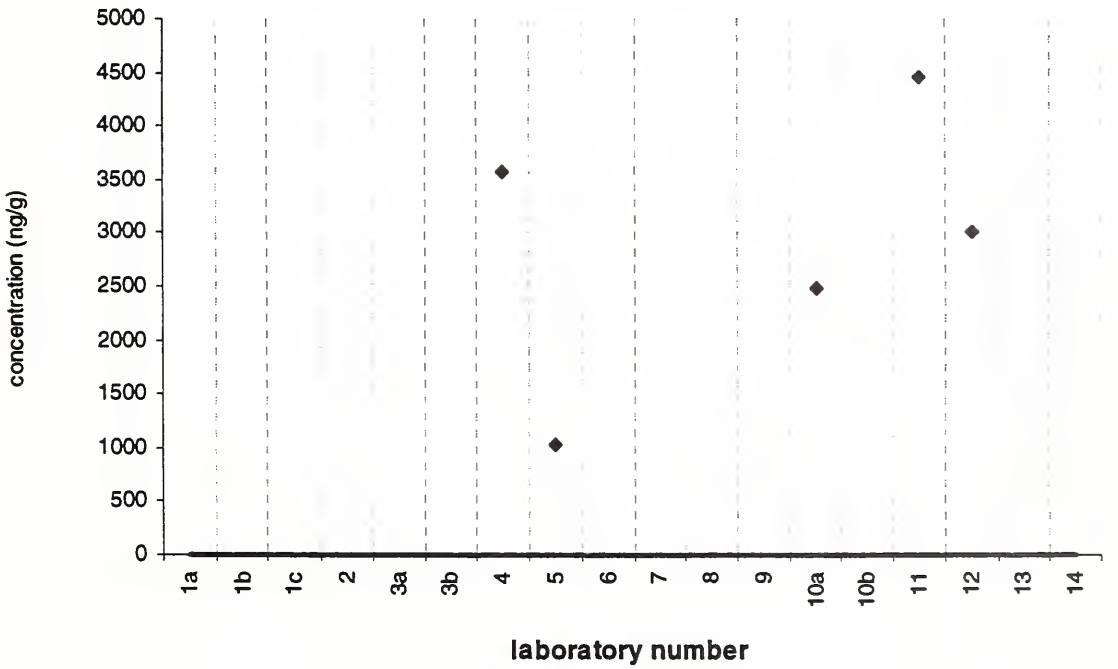


n-C21

SRM 1649a

Target Value = no target ng/g

Reported Results: 5 Quantitative Results: 5

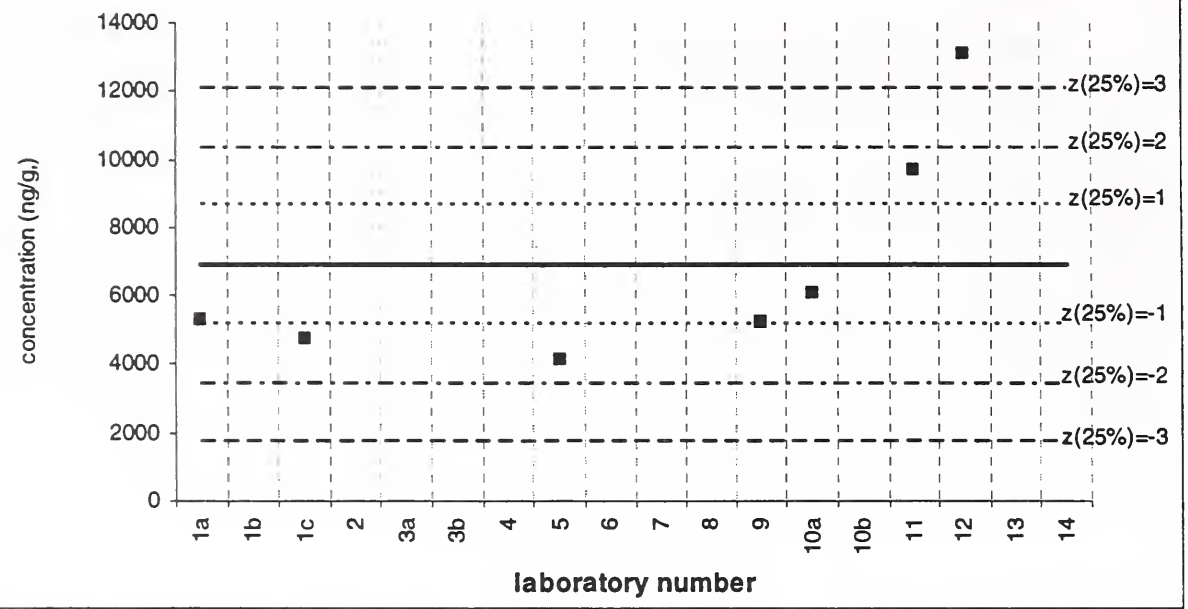


n-C22

SRM 1648

Assigned value (solid line) = 6898 ng/g s = 3268 ng/g 95% CL = 3022 ng/g

Reported Results: 7 Quantitative Results: 7

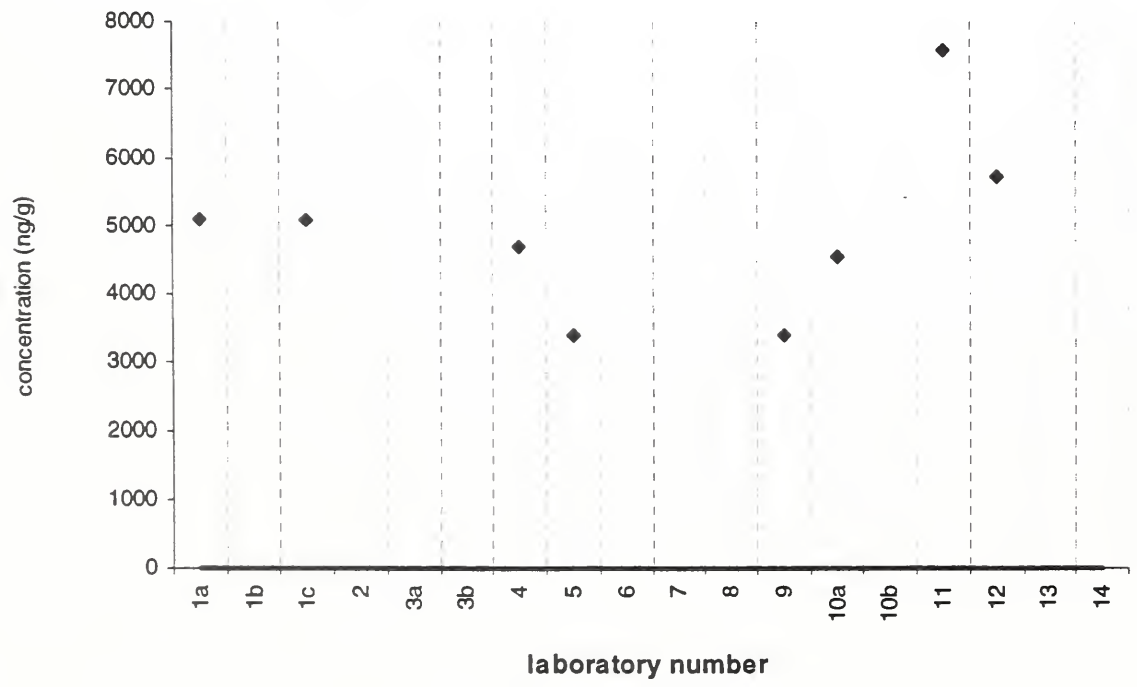


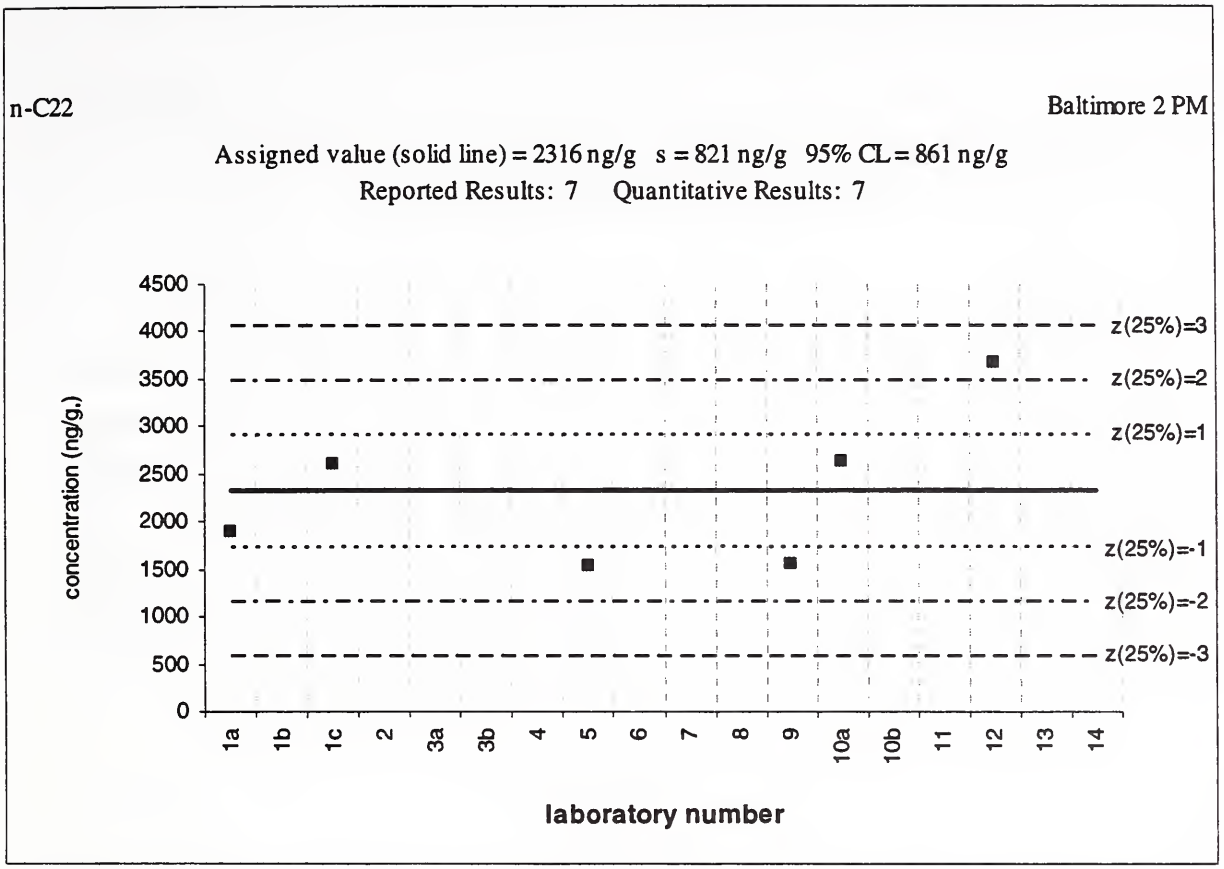
n-C22

SRM 1649a

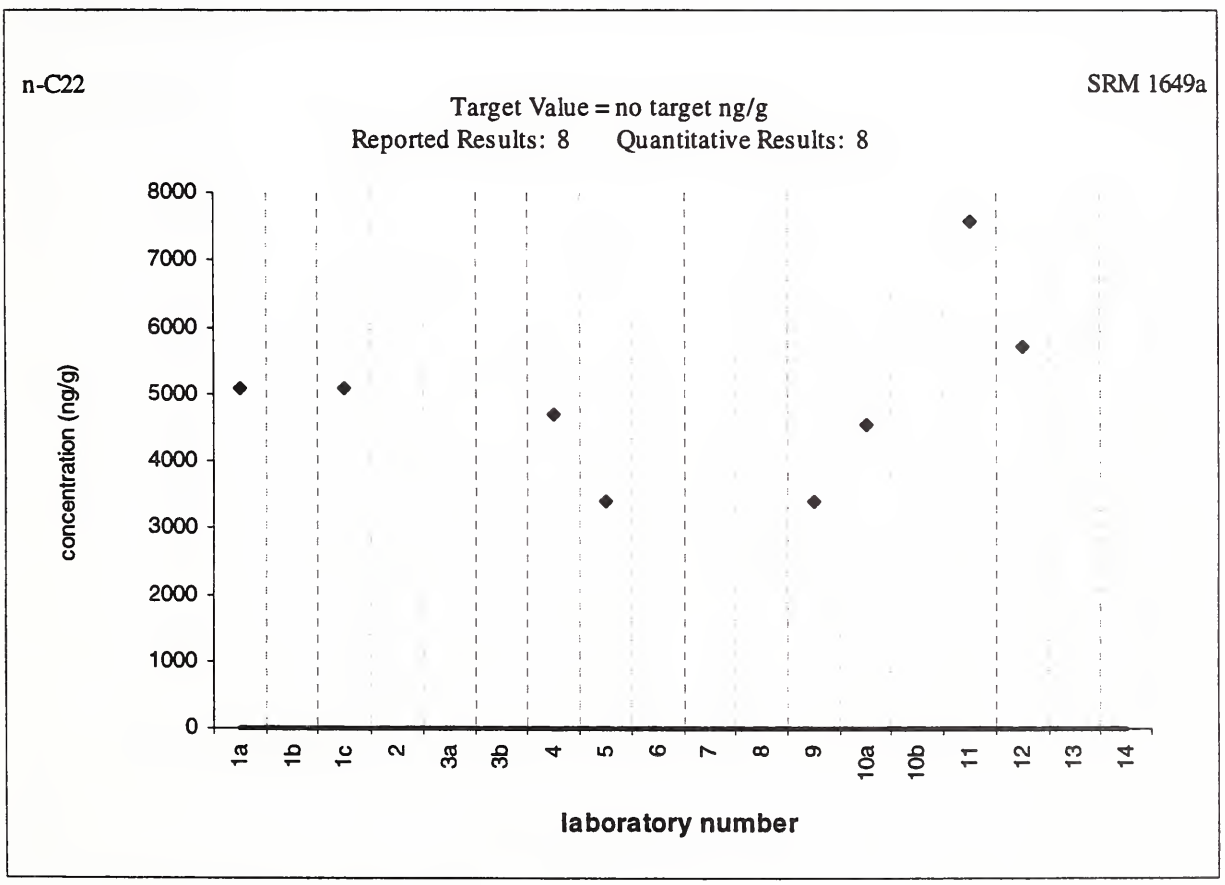
Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 8





lab 11 = 15794 ng/g

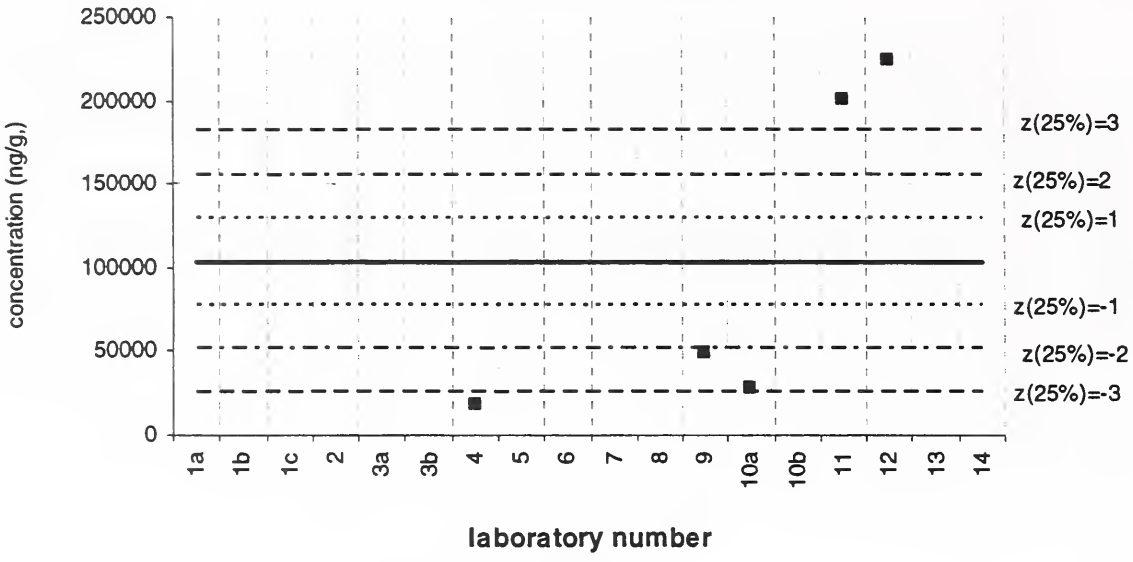


n-C22

Filter samples

Assigned value (solid line) = 103849 ng/g s = 99679 ng/g 95% CL = 123768 ng/g

Reported Results: 6 Quantitative Results: 5

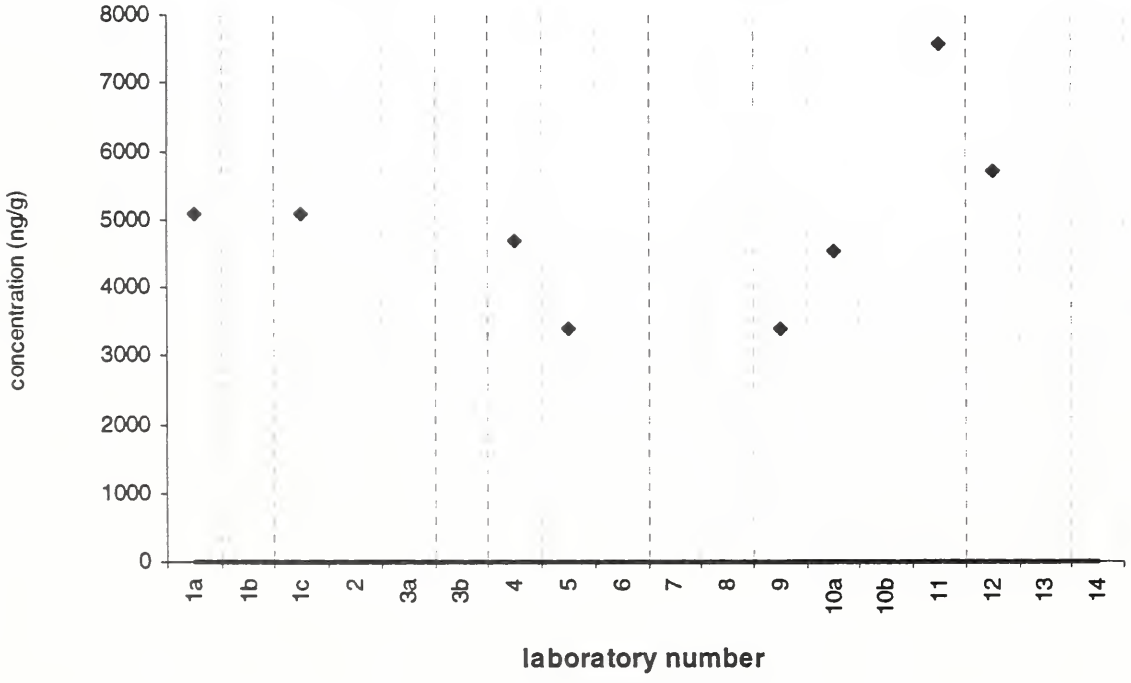


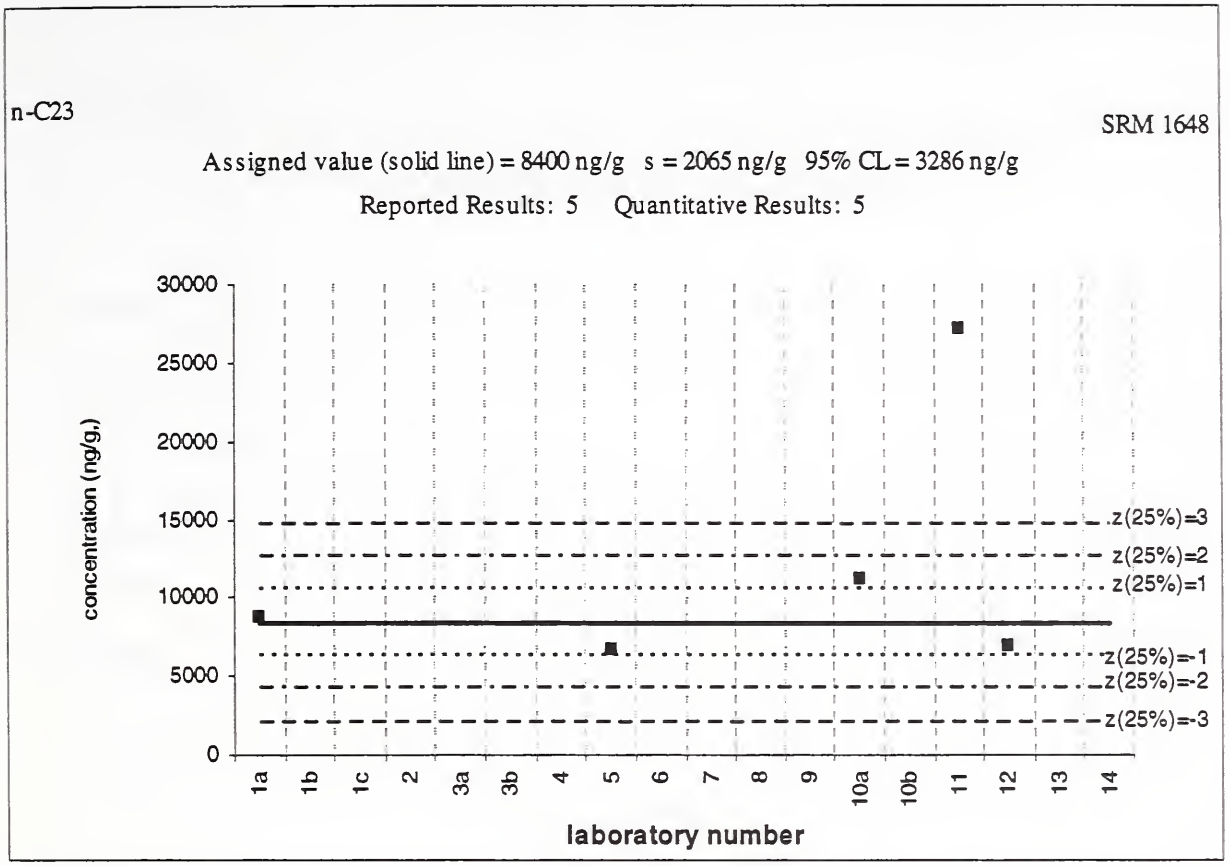
n-C22

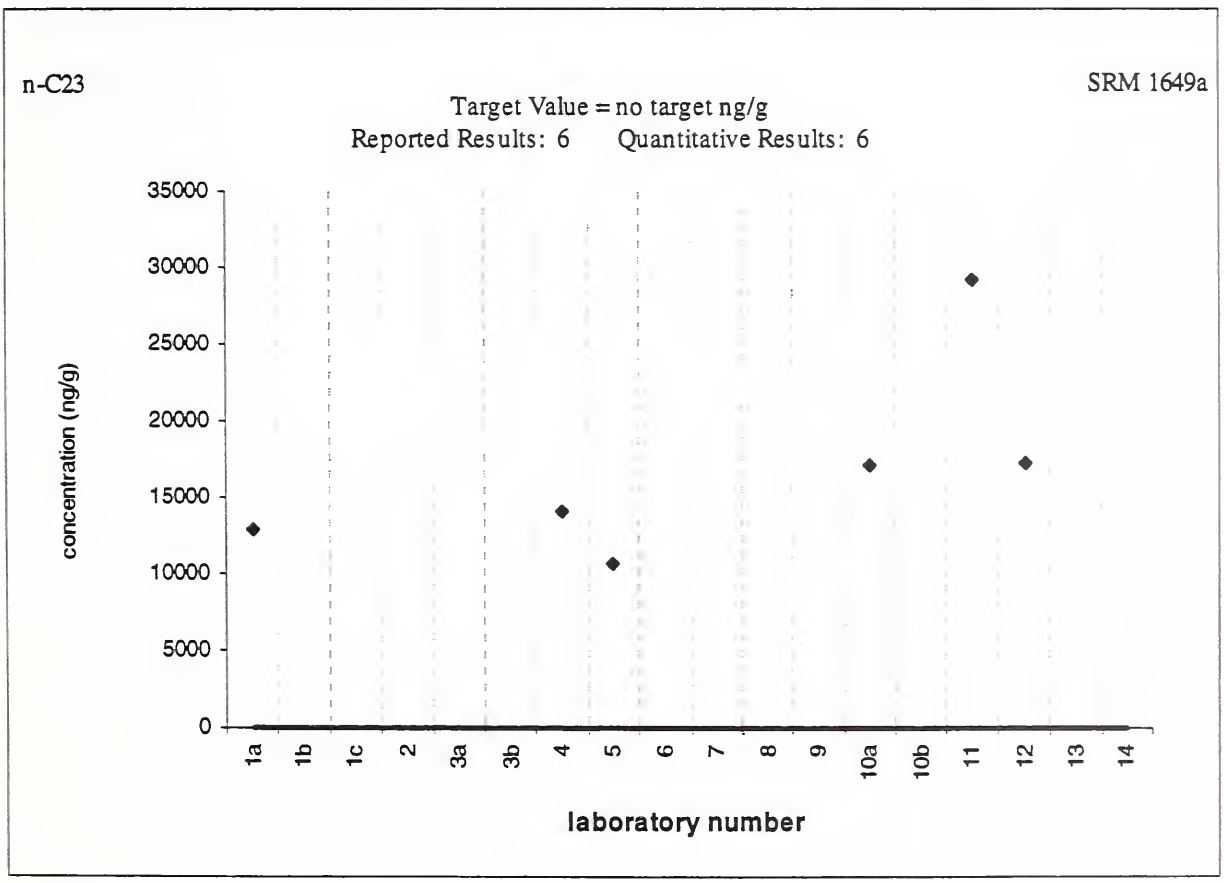
SRM 1649a

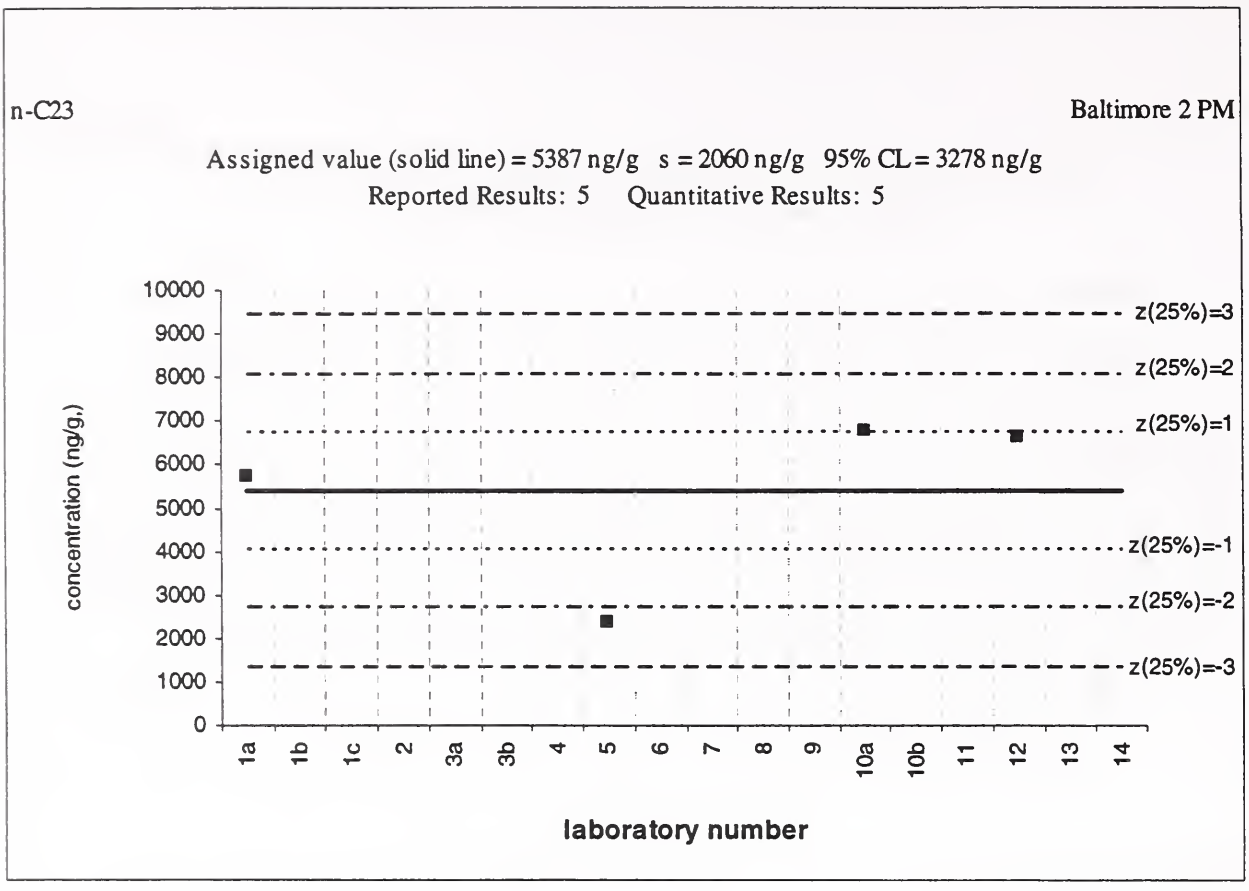
Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 8

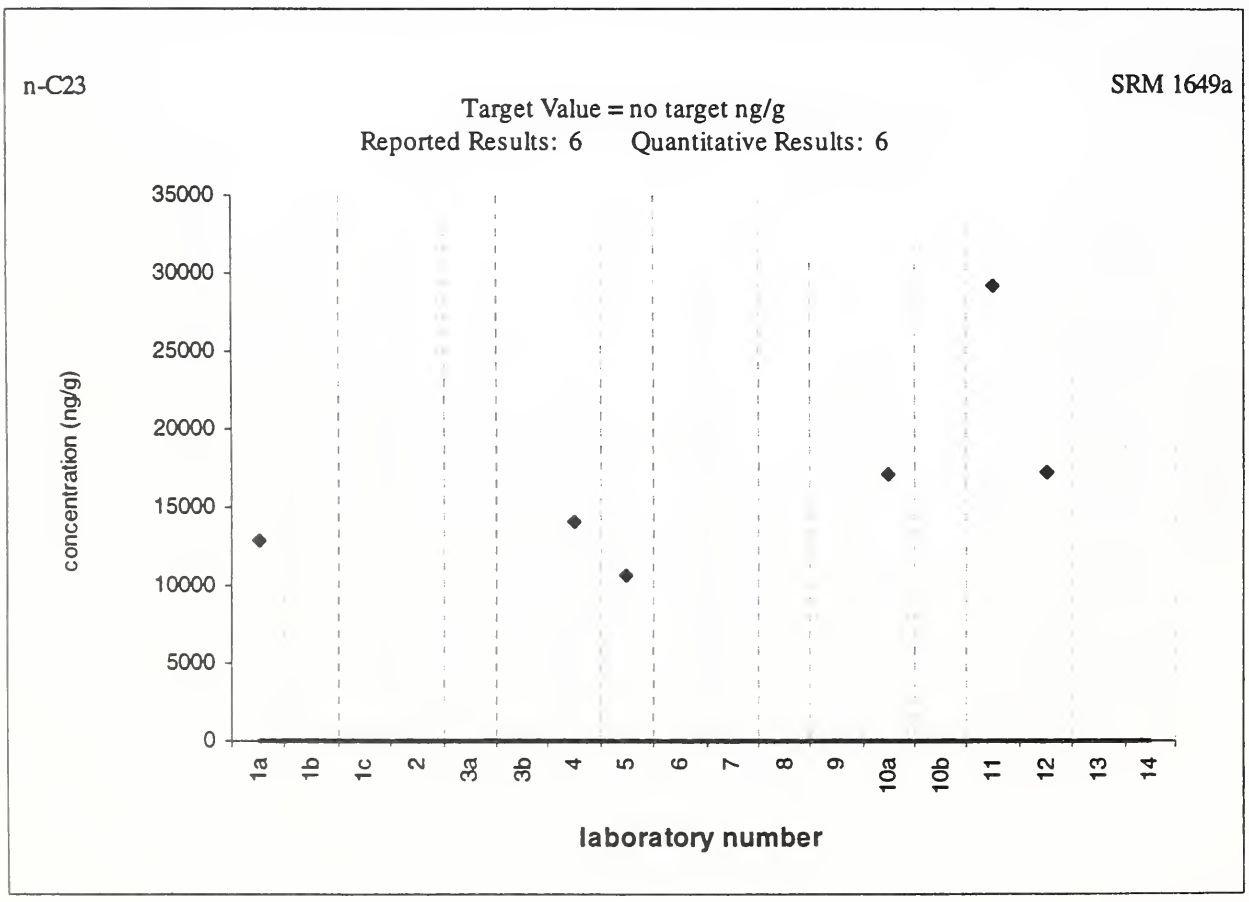


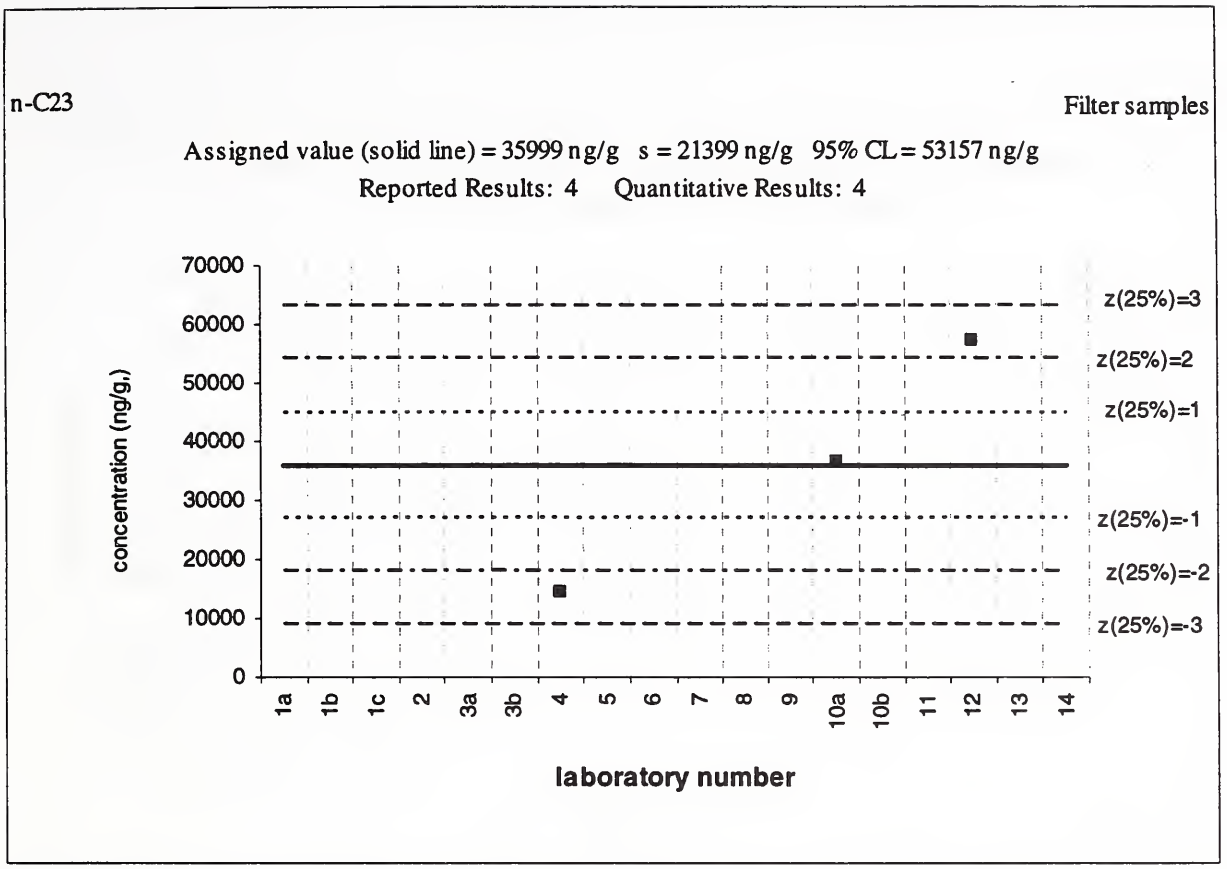

n-C23
SRM 1648
Assigned value (solid line) = 8400 ng/g s = 2065 ng/g 95% CL = 3286 ng/g
Reported Results: 5 Quantitative Results: 5
concentration (ng/g)
30000
25000
20000
15000
10000
5000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number


n-C23
SRM 1649a
Target Value = no target ng/g
Reported Results: 6 Quantitative Results: 6
concentration (ng/g)
35000
30000
25000
20000
15000
10000
5000
0
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

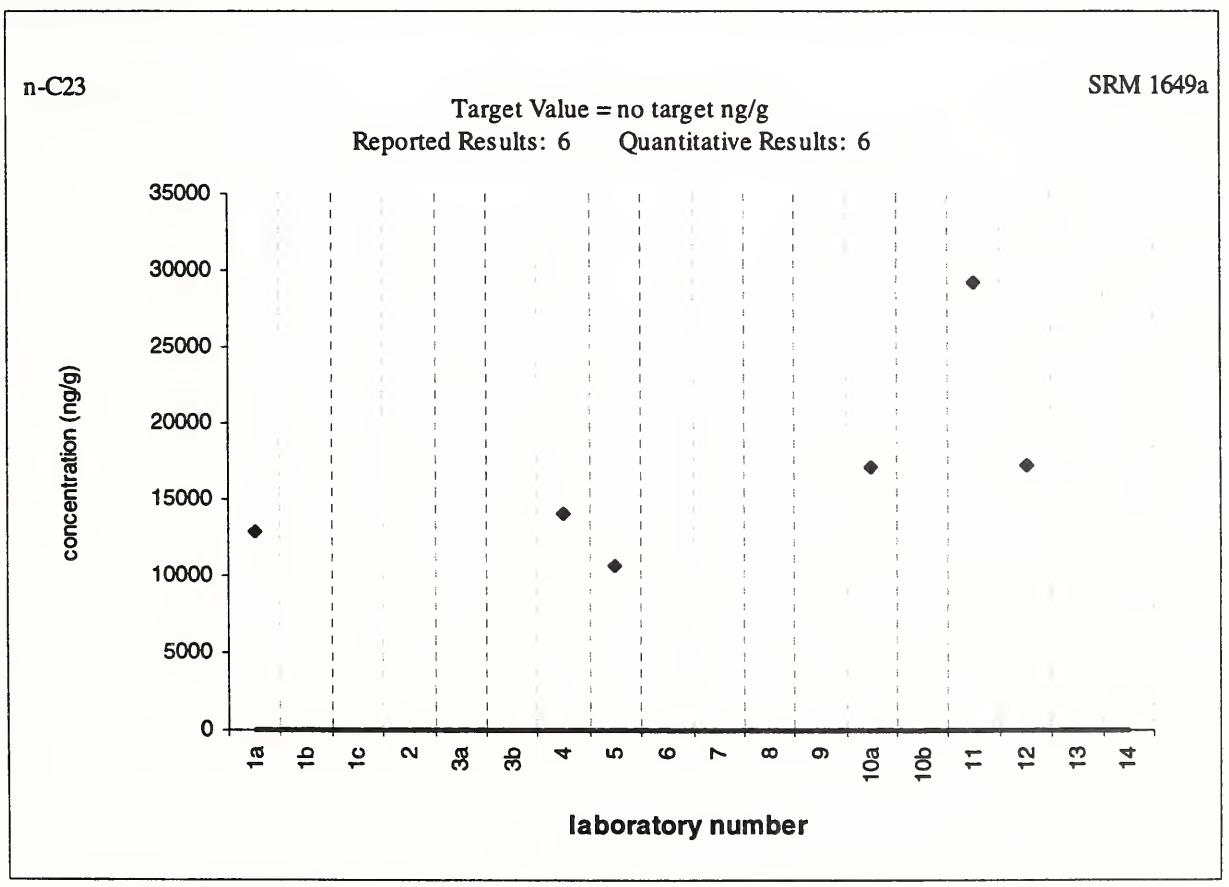


lab 11 = 64816 ng/g





lab 11 = 367237 ng/g

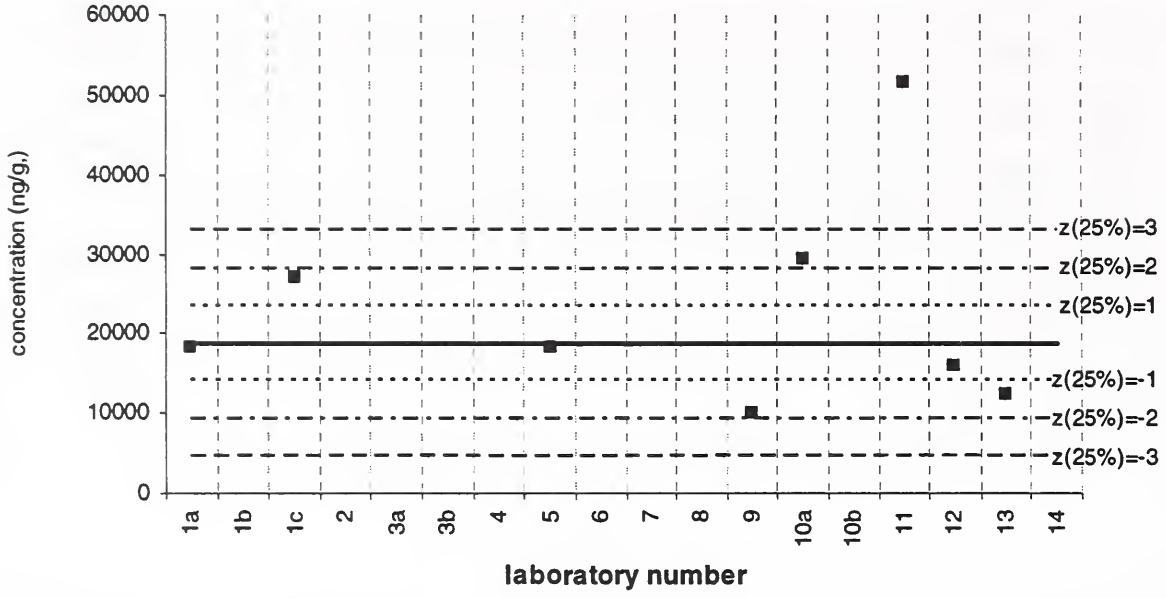


n-C24

SRM 1648

Assigned value (solid line) = 18762 ng/g s = 7130 ng/g 95% CL = 5961 ng/g

Reported Results: 8 Quantitative Results: 8

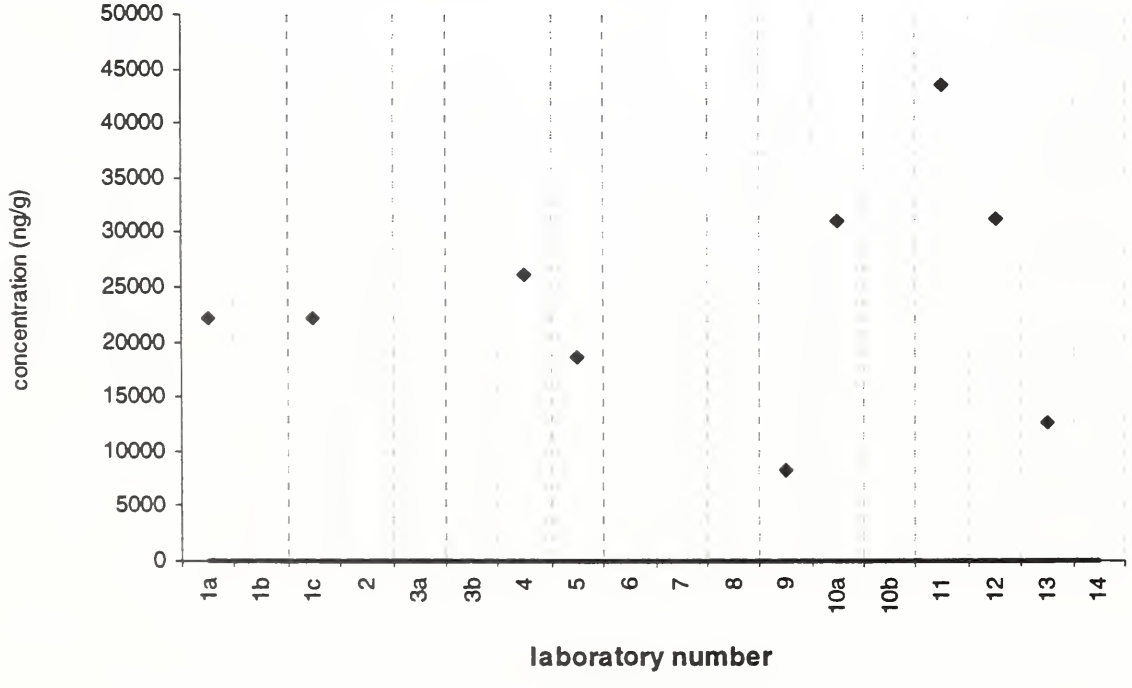


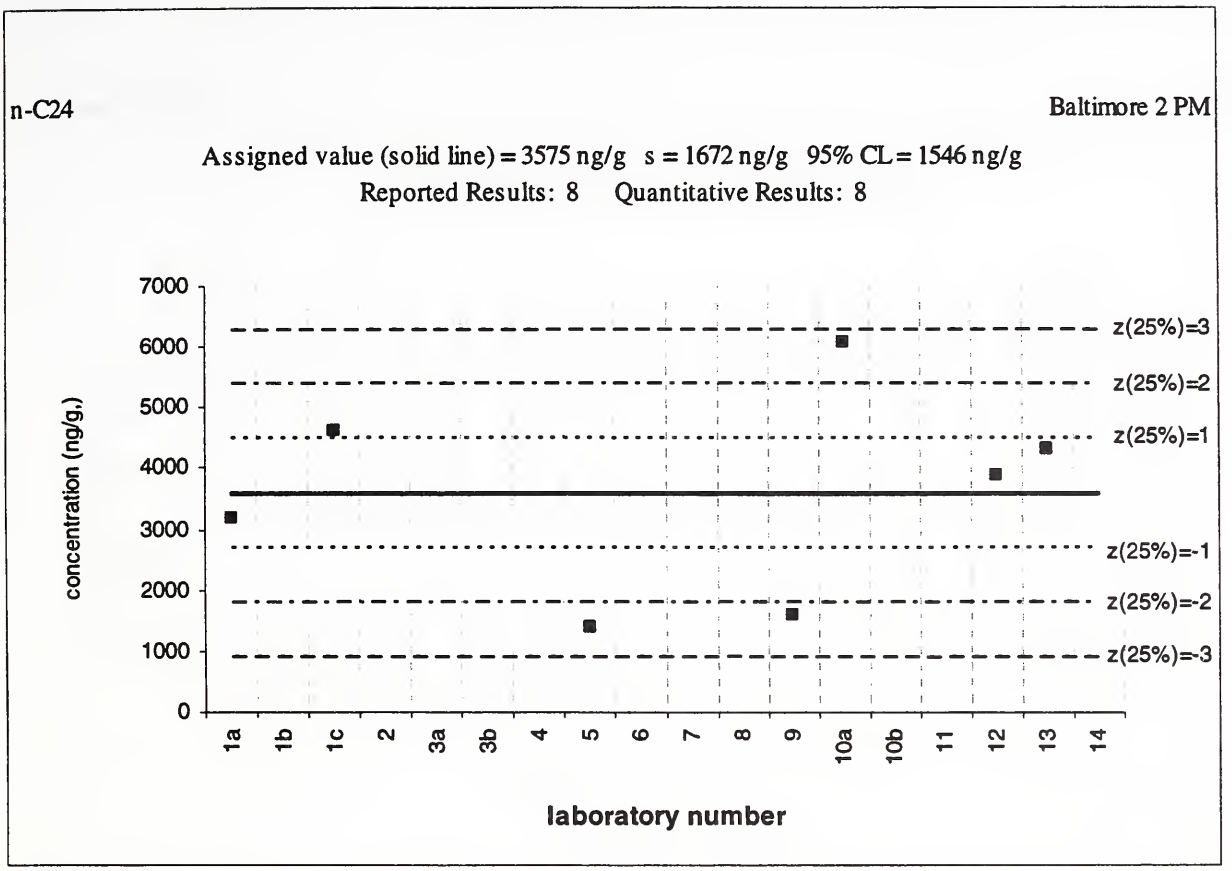
n-C24

SRM 1649a

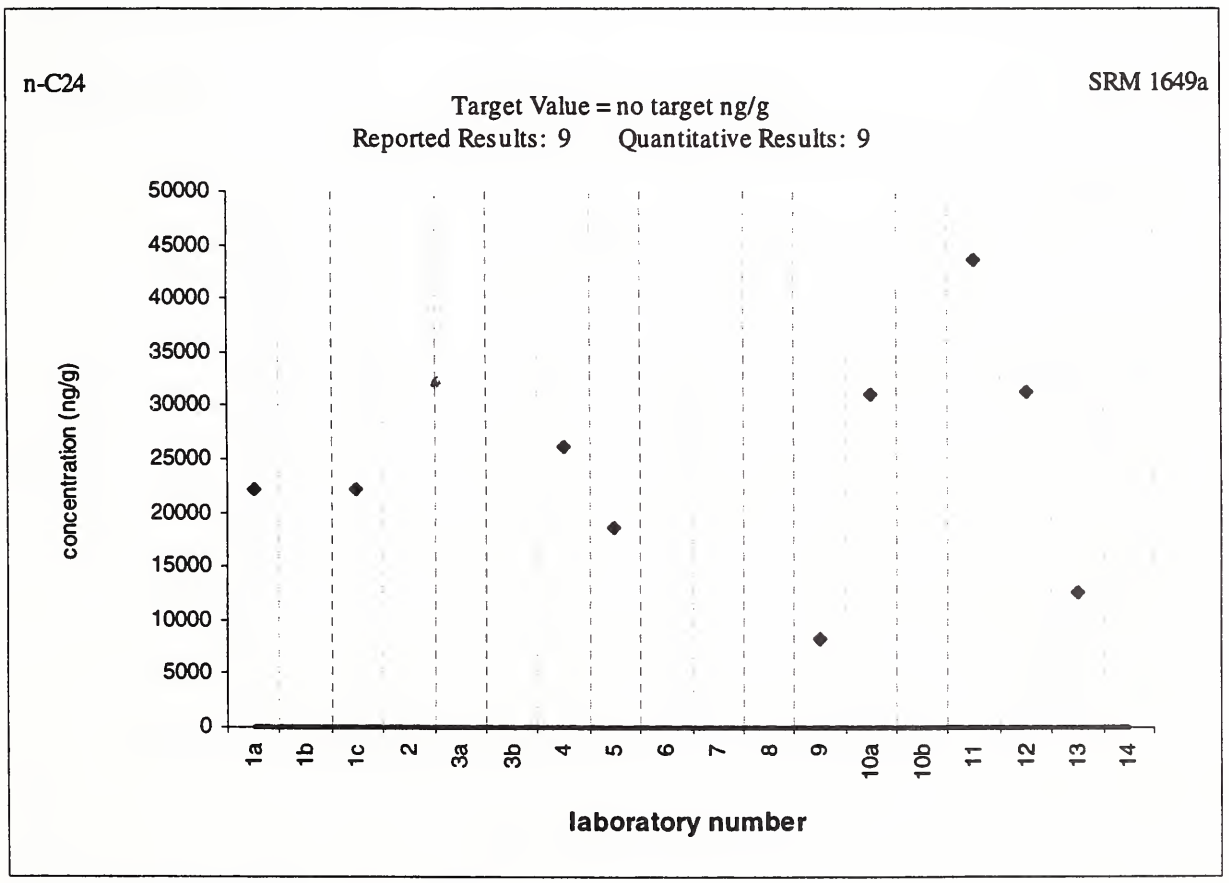
Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9





lab 11 = 51000 ng/g

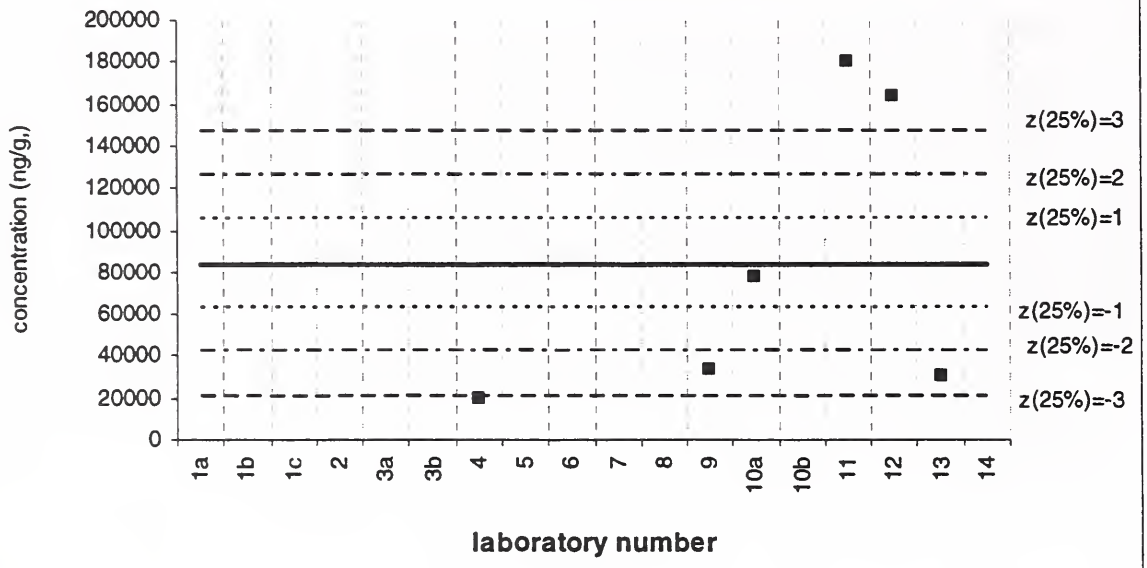


n-C24

Filter samples

Assigned value (solid line) = 84067 ng/g s = 70739 ng/g 95% CL = 74236 ng/g

Reported Results: 7 Quantitative Results: 6

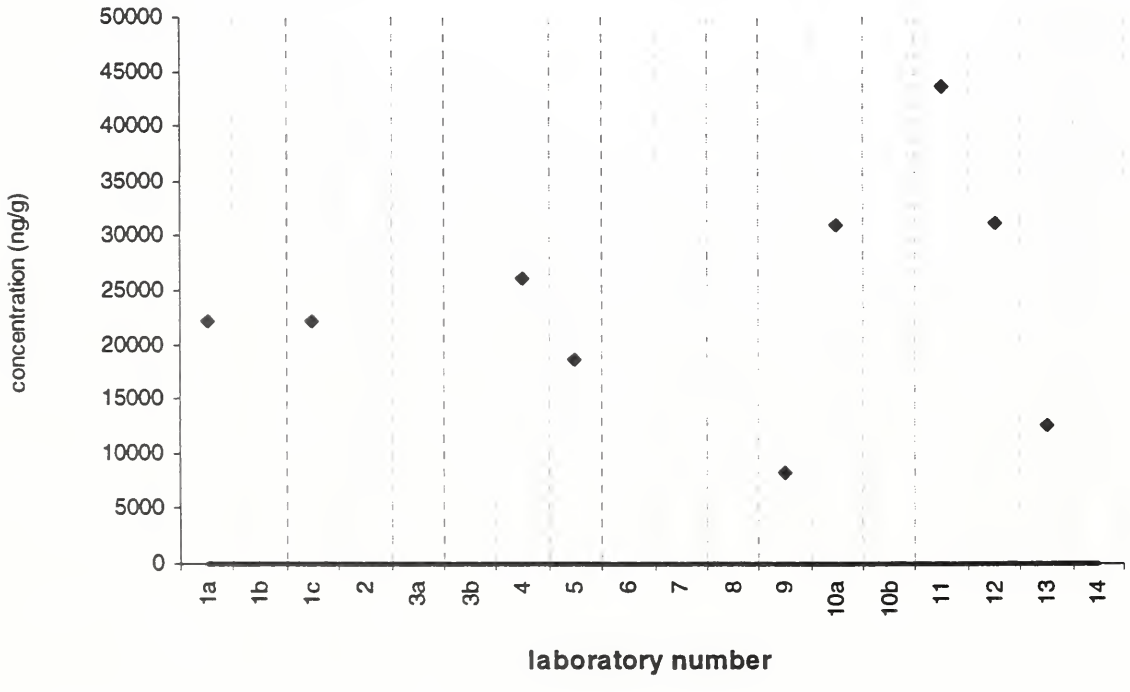


n-C24

SRM 1649a

Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9

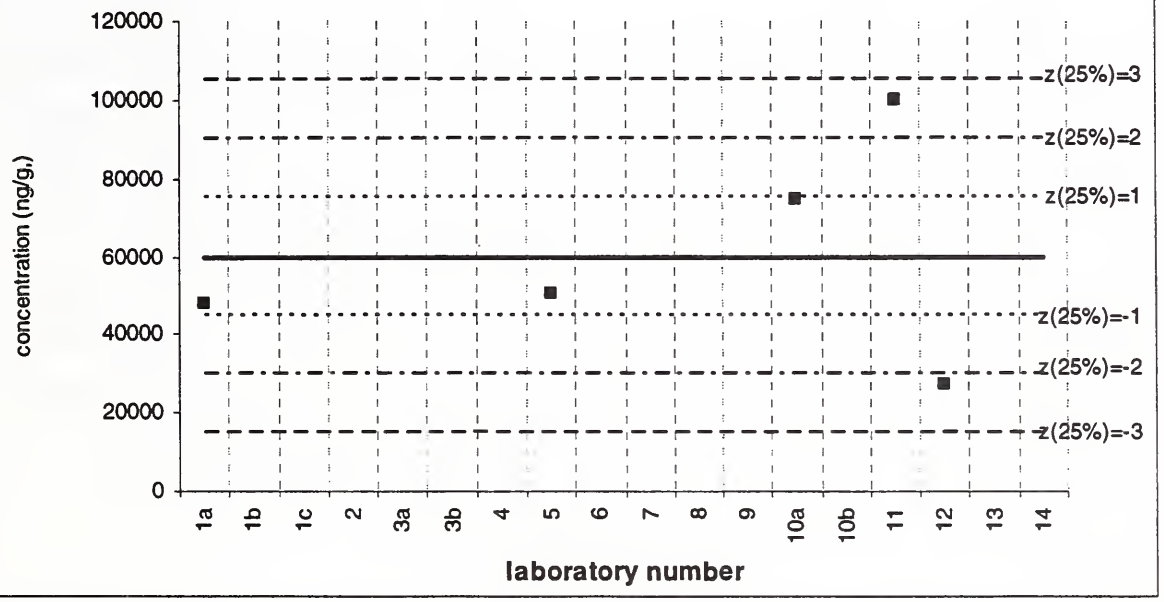


n-C25

SRM 1648

Assigned value (solid line) = 59986 ng/g s = 28043 ng/g 95% CL = 34820 ng/g

Reported Results: 5 Quantitative Results: 5

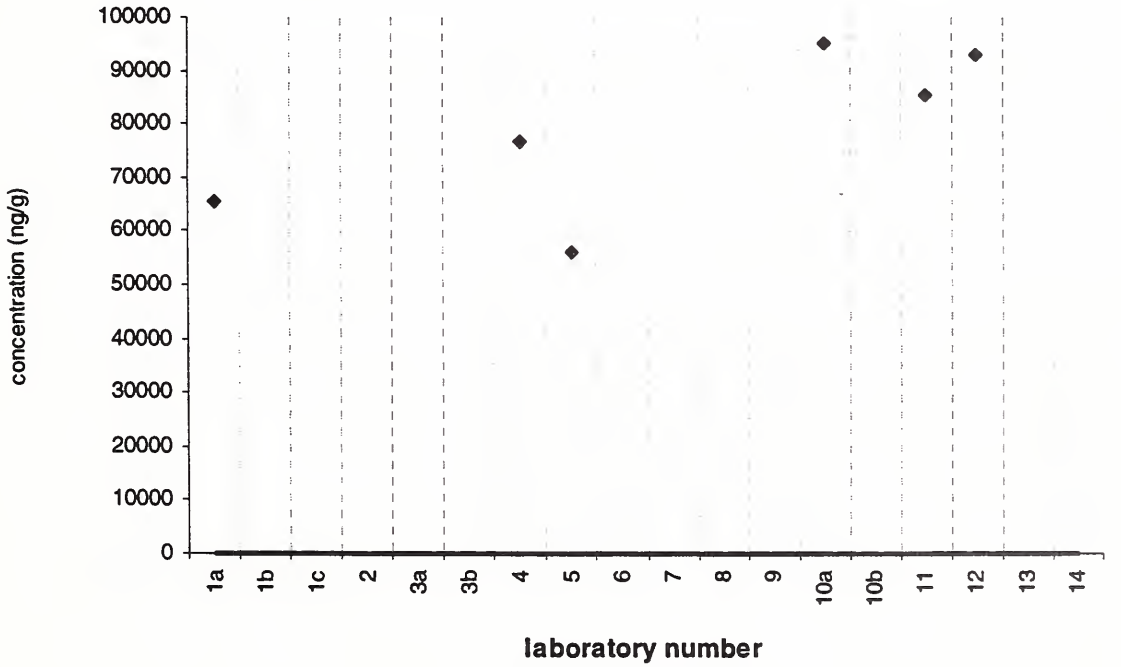


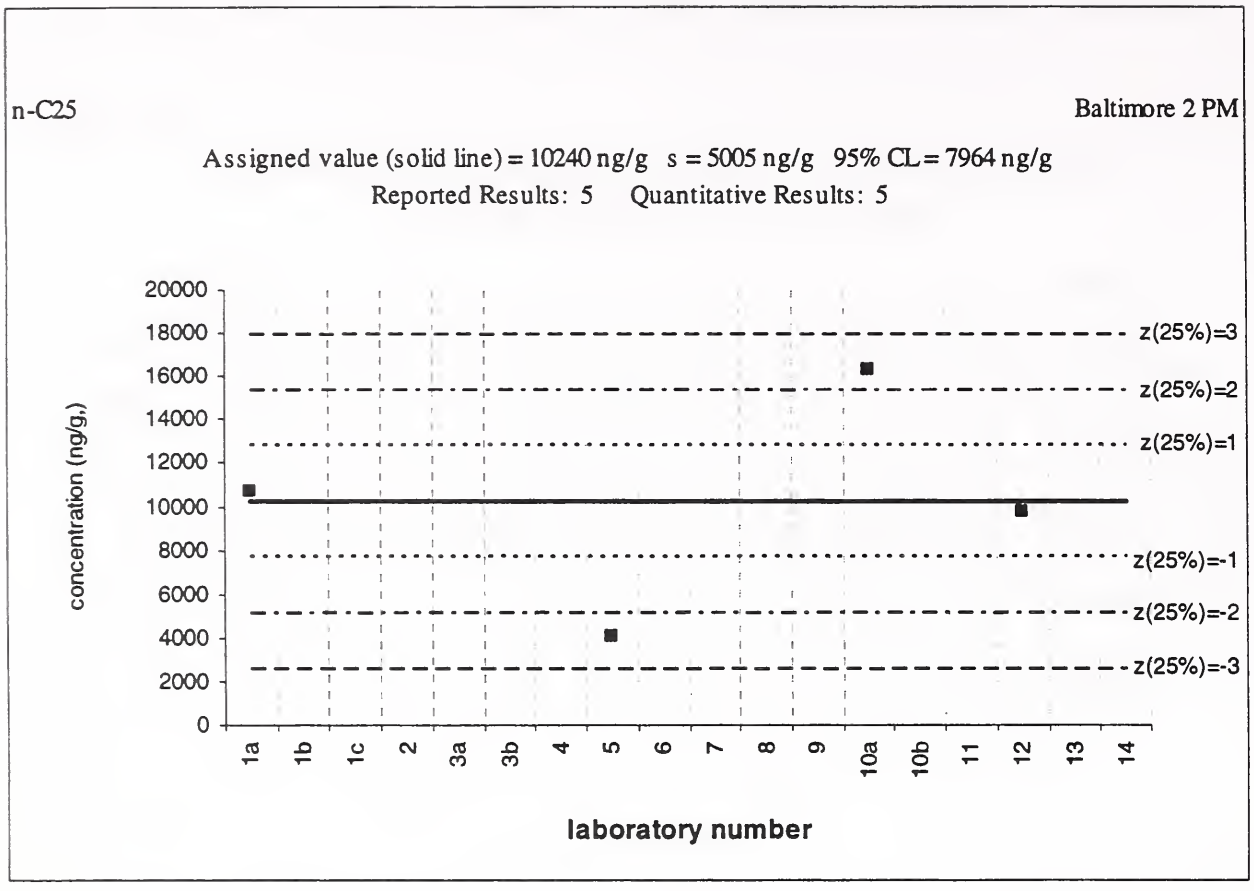
n-C25

SRM 1649a

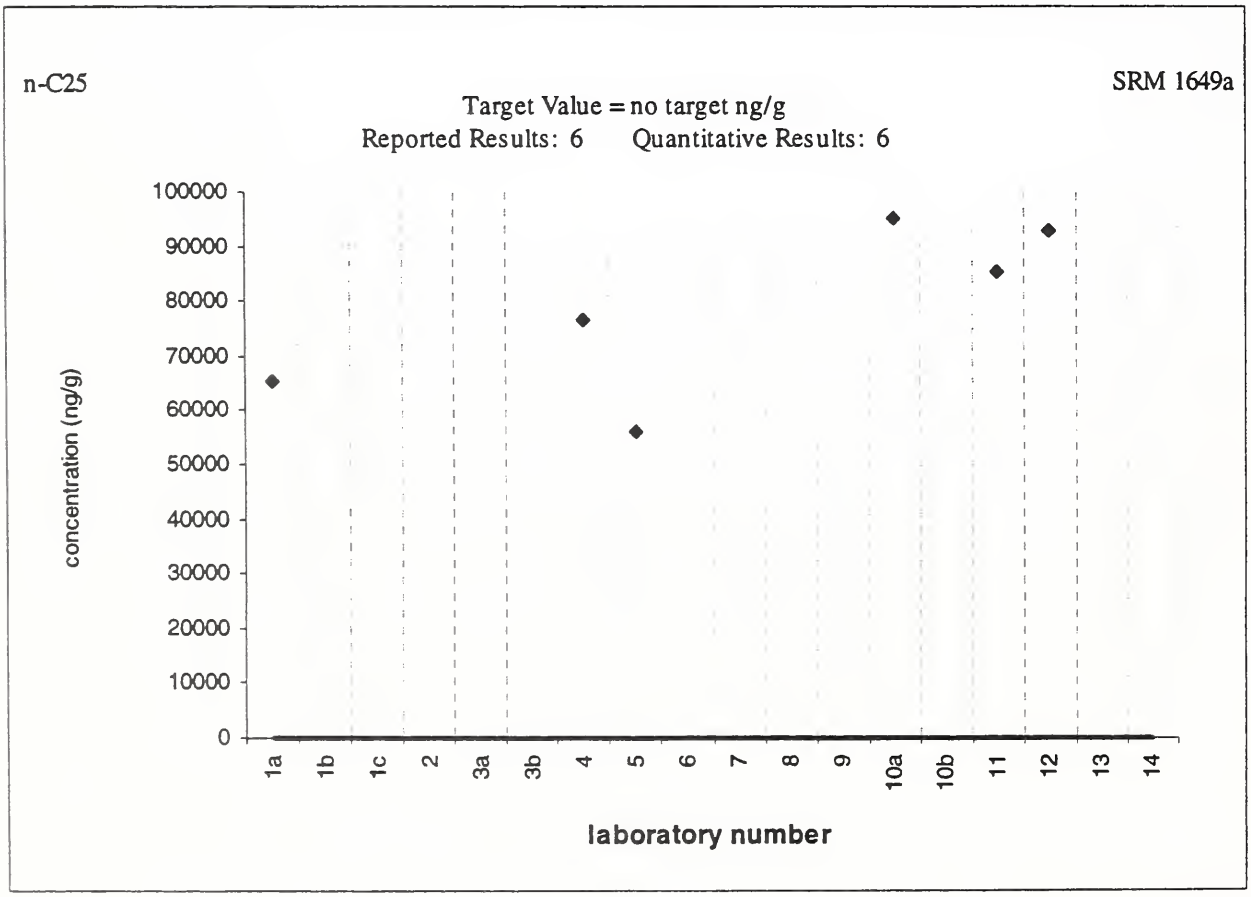
Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6





lab 11 = 59841 ng/g

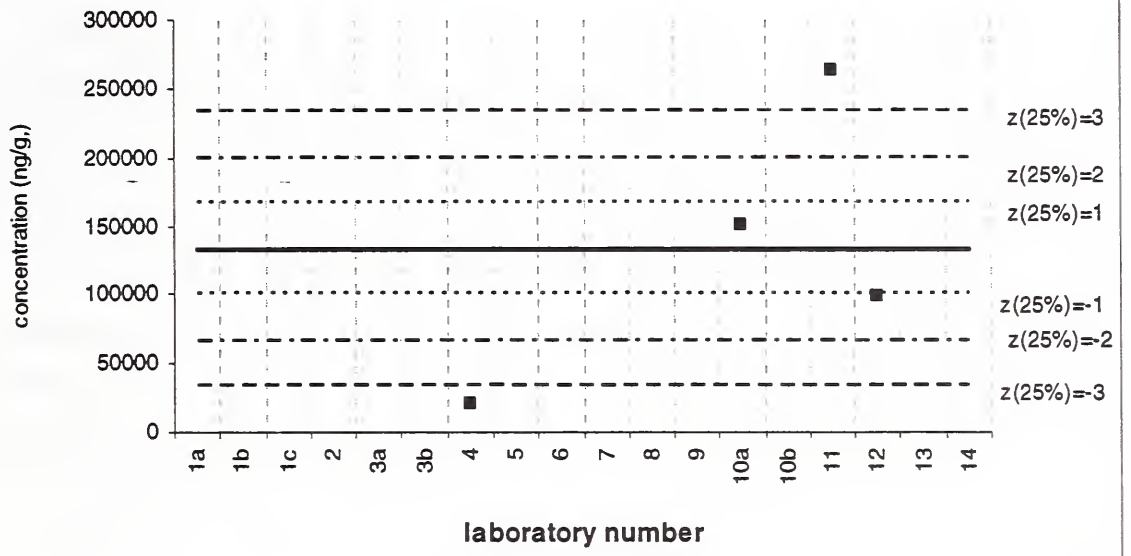


n-C25

Filter samples

Assigned value (solid line) = 133314 ng/g s = 101428 ng/g 95% CL = 161395 ng/g

Reported Results: 4 Quantitative Results: 4

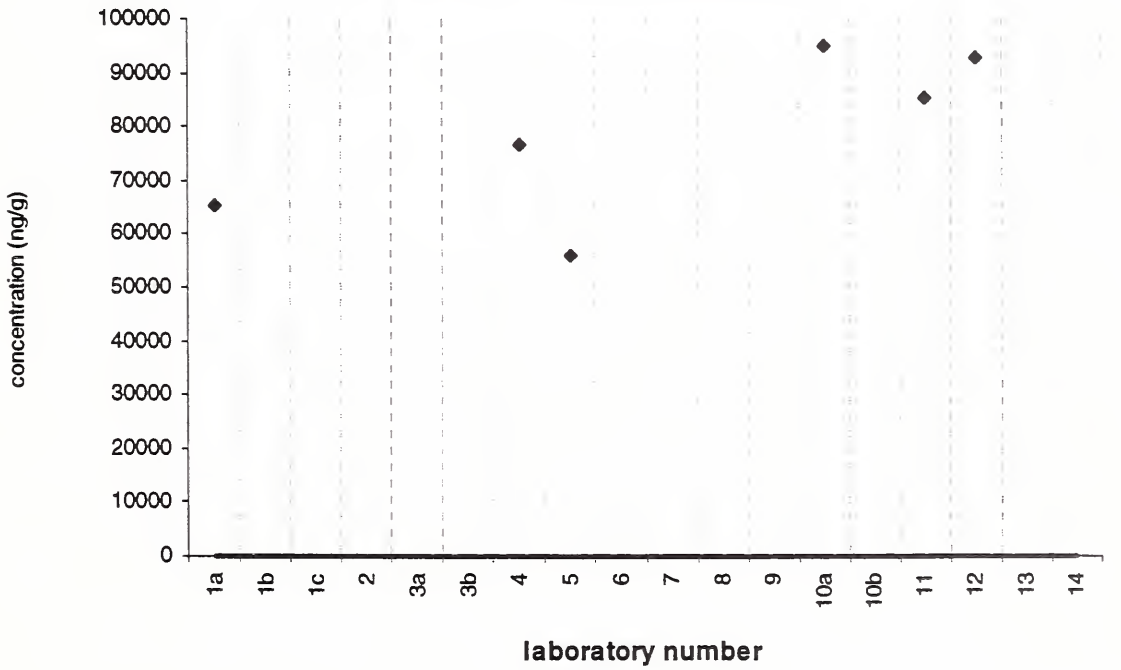


n-C25

SRM 1649a

Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6

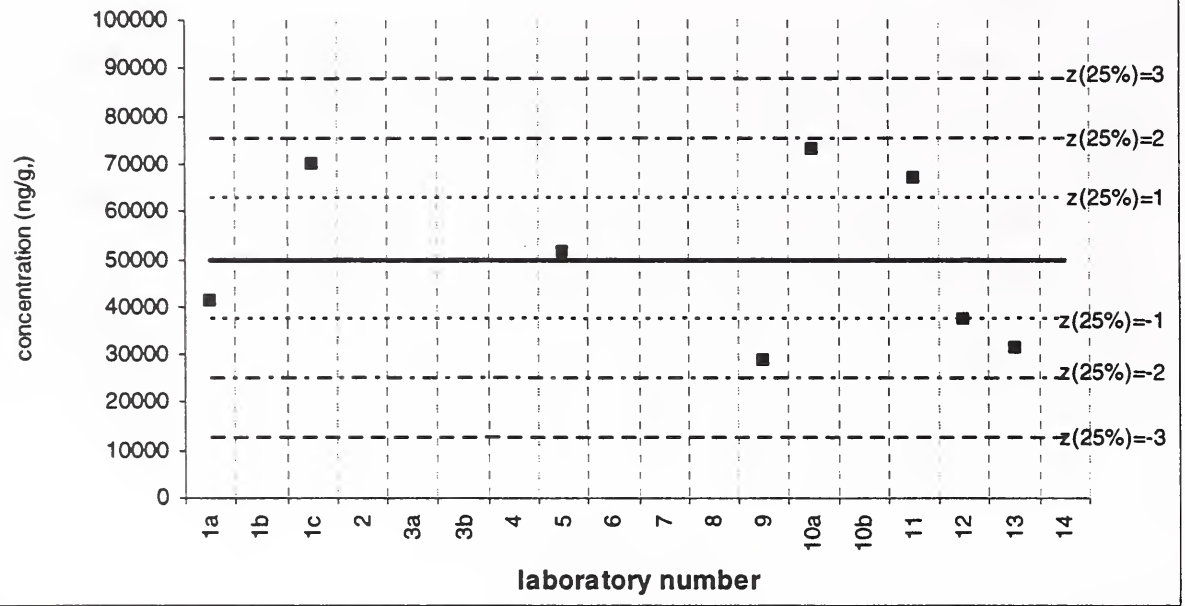


n-C26

SRM 1648

Assigned value (solid line) = 49986 ng/g s = 17838 ng/g 95% CL = 14913 ng/g

Reported Results: 8 Quantitative Results: 8

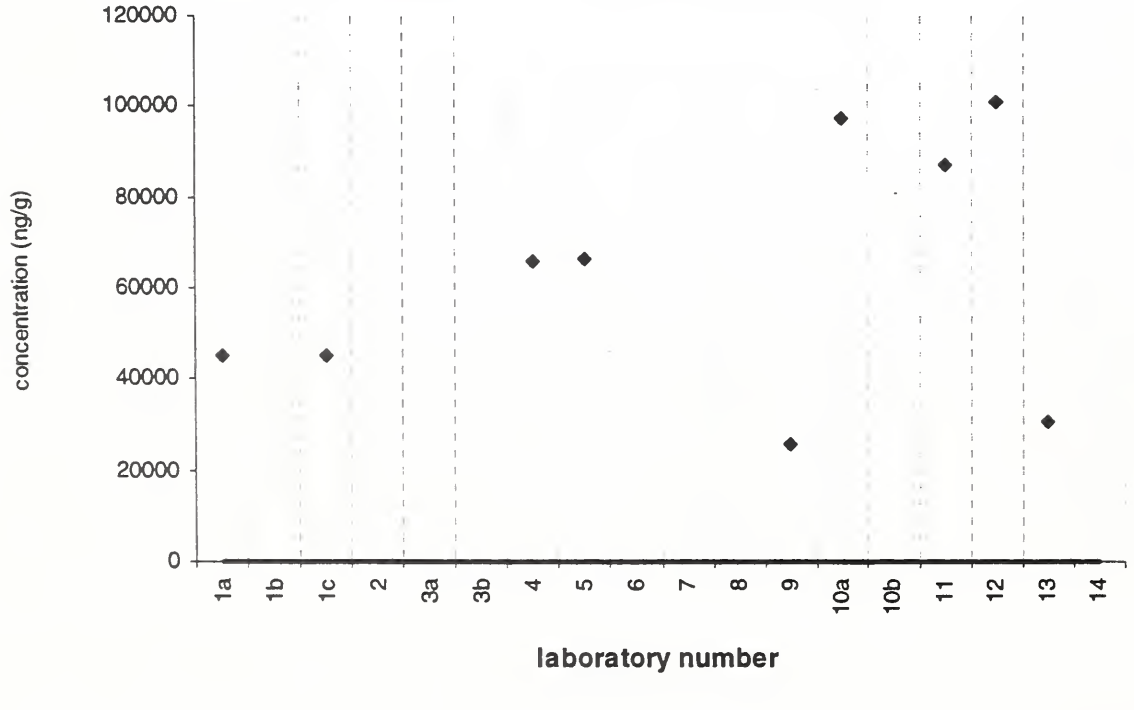


n-C26

SRM 1649a

Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9

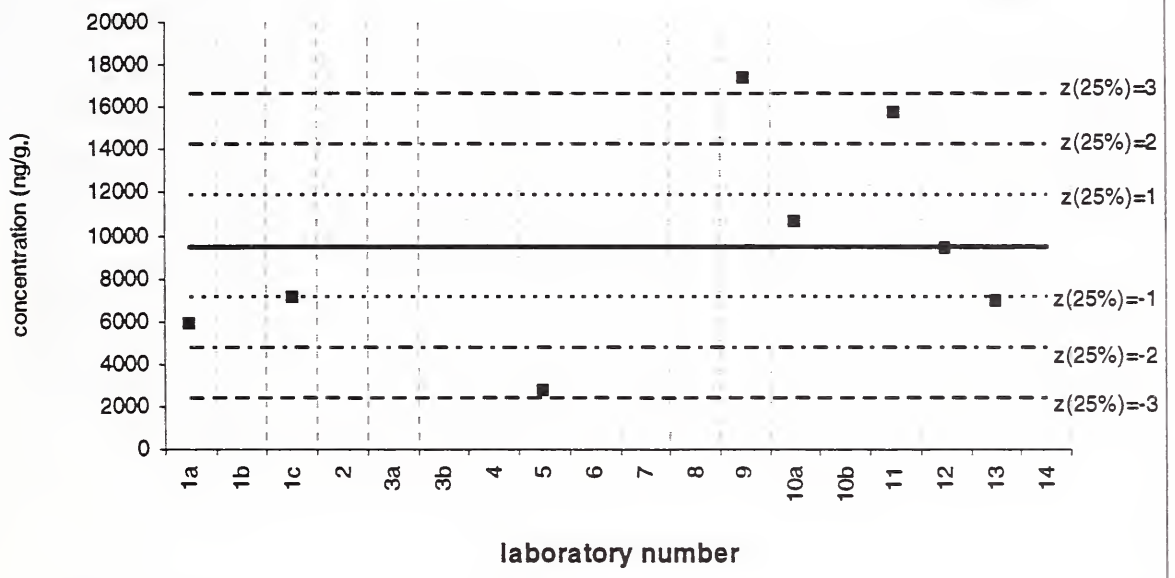


n-C26

Baltimore 2 PM

Assigned value (solid line) = 9465 ng/g s = 4967 ng/g 95% CL = 4152 ng/g

Reported Results: 8 Quantitative Results: 8

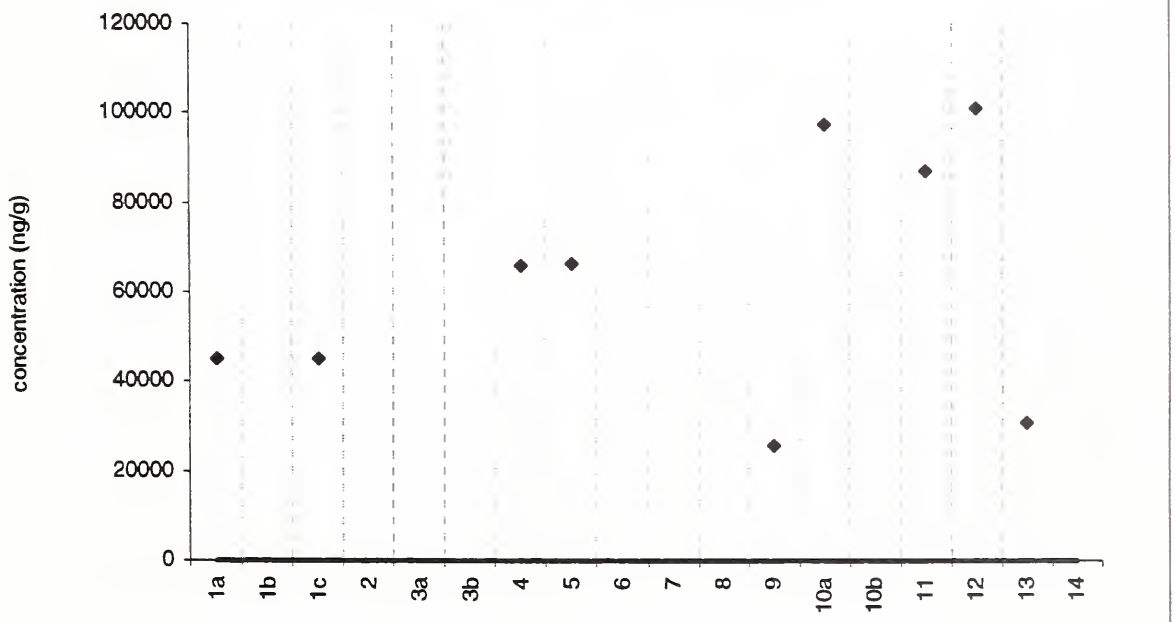


n-C26

SRM 1649a

Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9

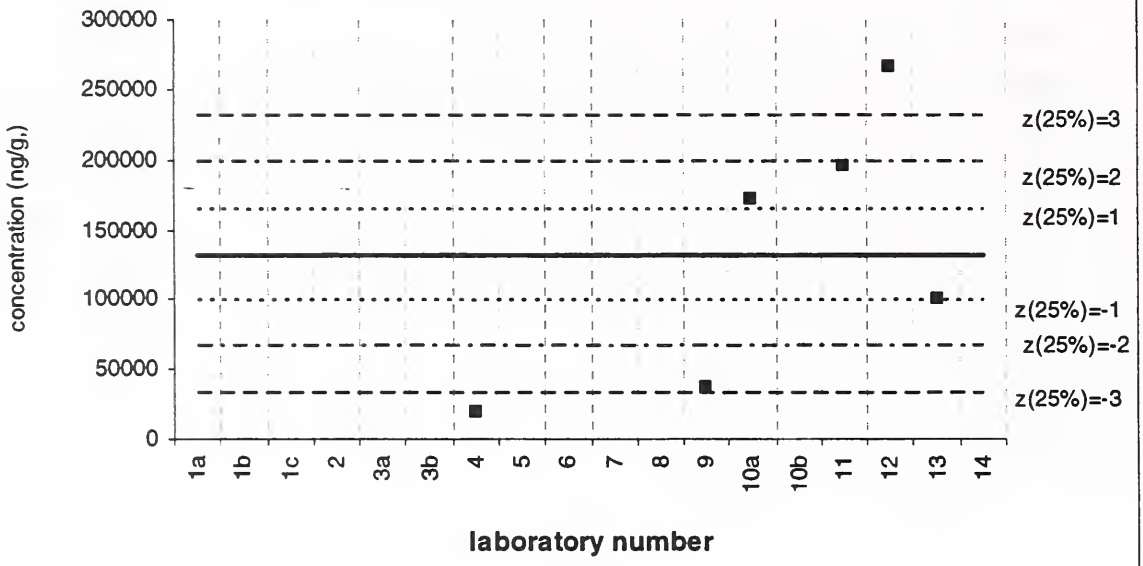


n-C26

Filter samples

Assigned value (solid line) = 131565 ng/g s = 96266 ng/g 95% CL = 101025 ng/g

Reported Results: 7 Quantitative Results: 6

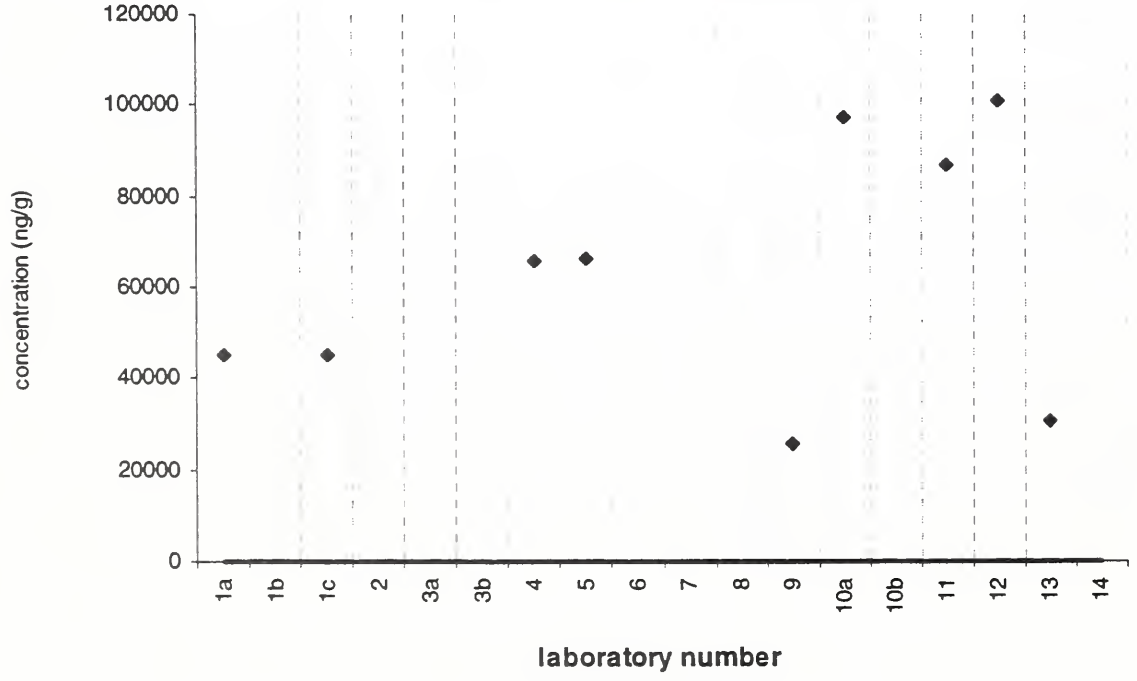


n-C26

SRM 1649a

Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9

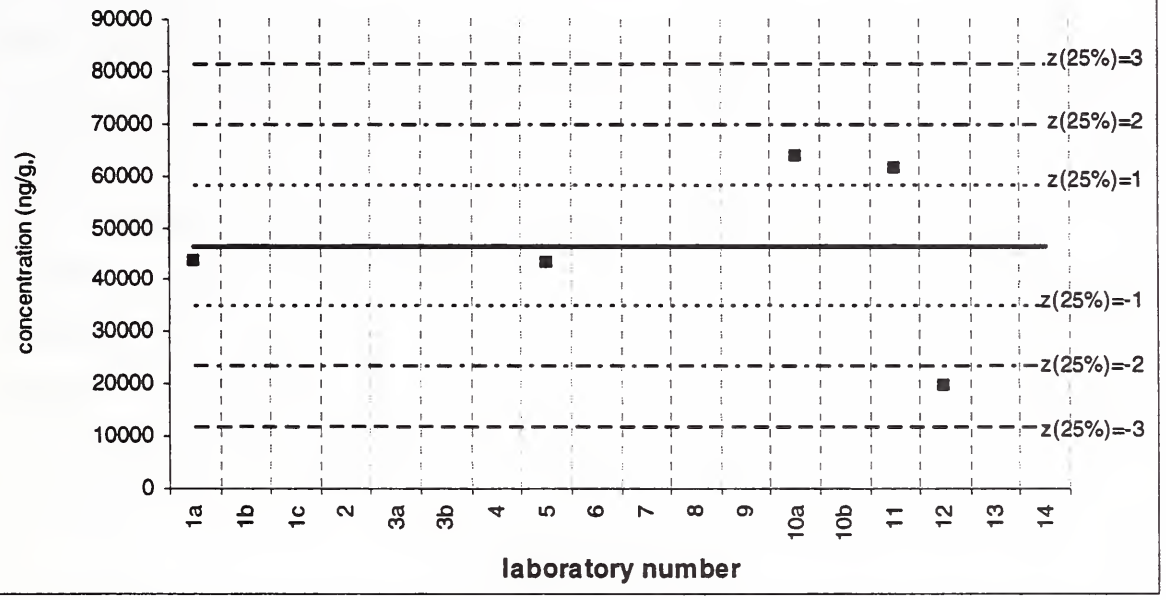


n-C27

SRM 1648

Assigned value (solid line) = 46332 ng/g s = 17656 ng/g 95% CL = 21923 ng/g

Reported Results: 5 Quantitative Results: 5

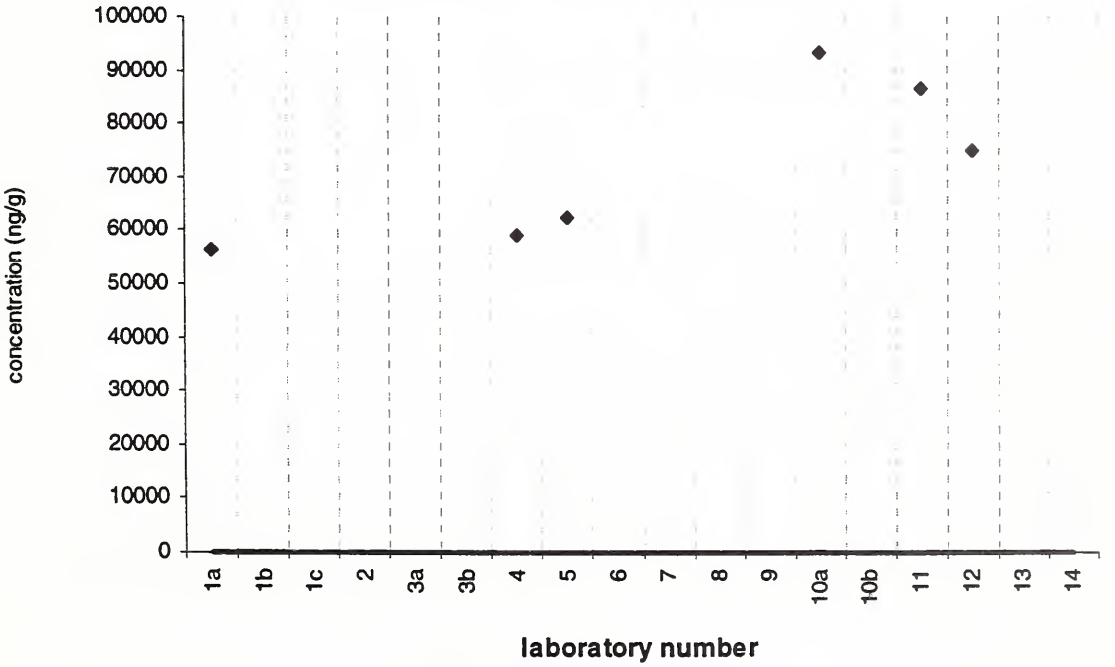


n-C27

SRM 1649a

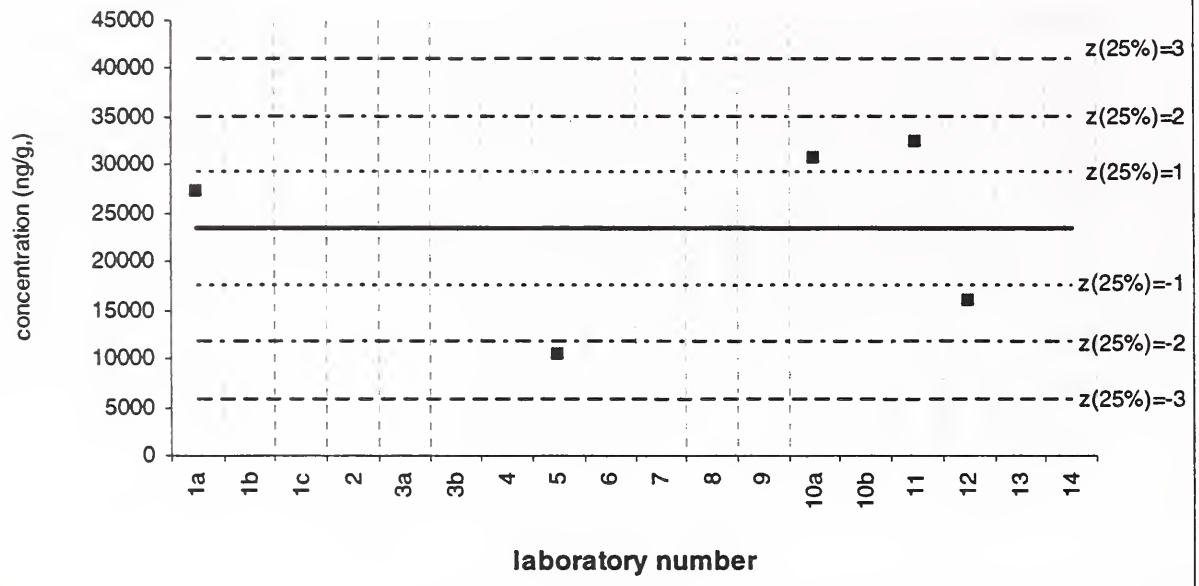
Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6



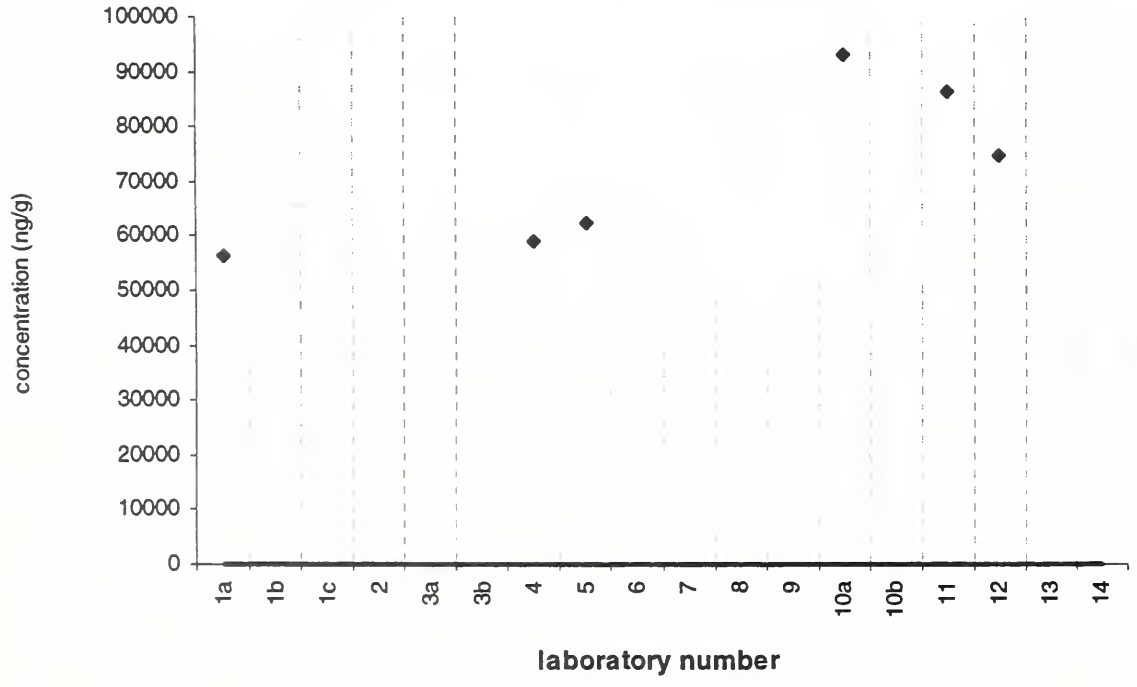
n-C27 Baltimore 2 PM

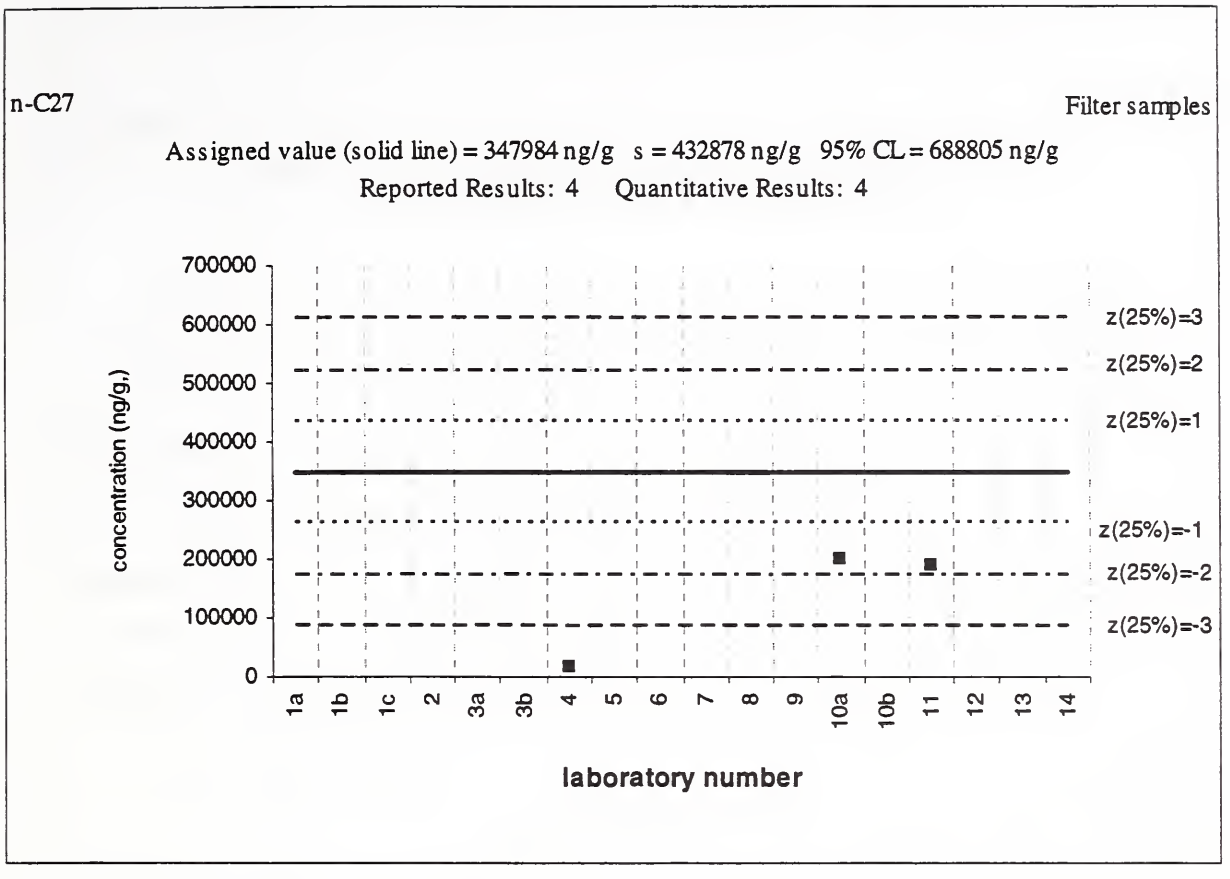
Assigned value (solid line) = 23370 ng/g s = 9629 ng/g 95% CL = 11956 ng/g
Reported Results: 5 Quantitative Results: 5



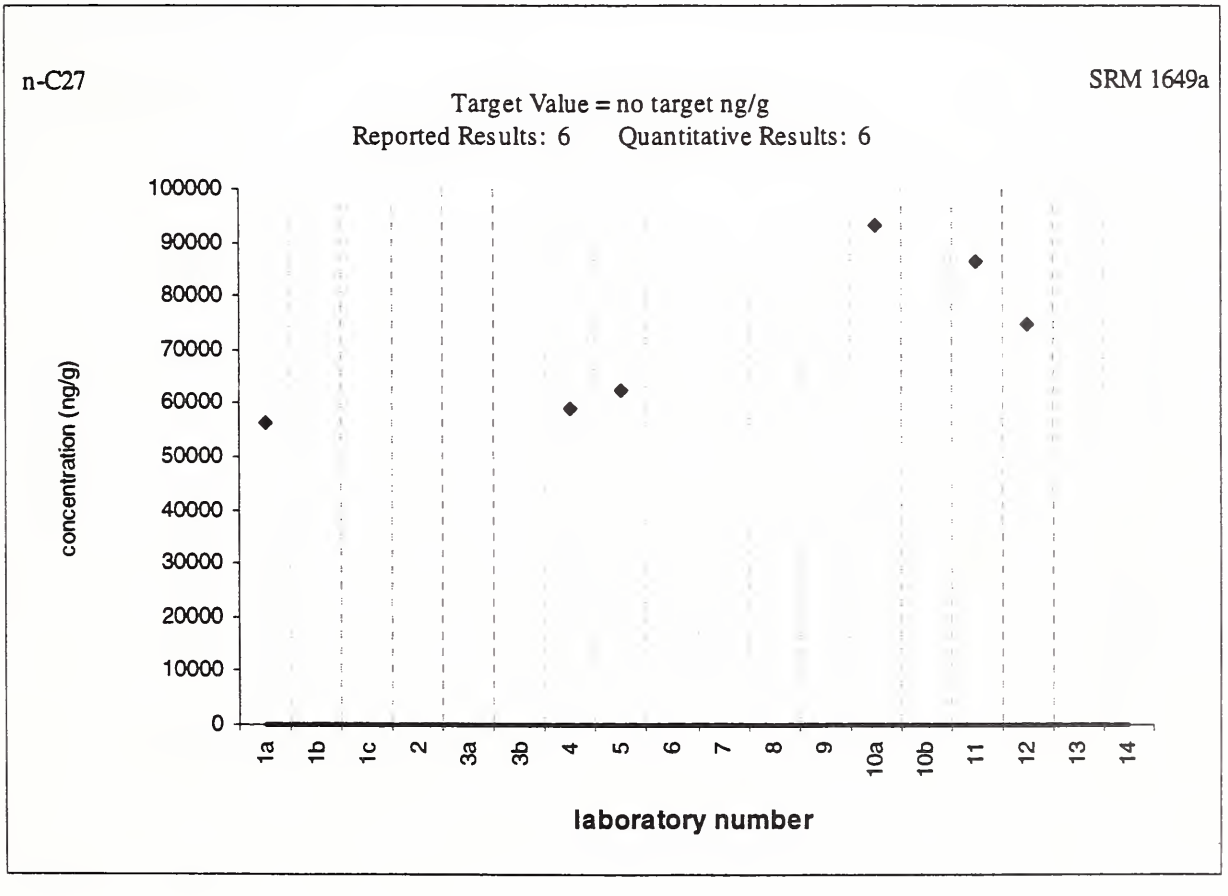
n-C27 SRM 1649a

Target Value = no target ng/g
Reported Results: 6 Quantitative Results: 6





lab 12 = 985305 ng/g

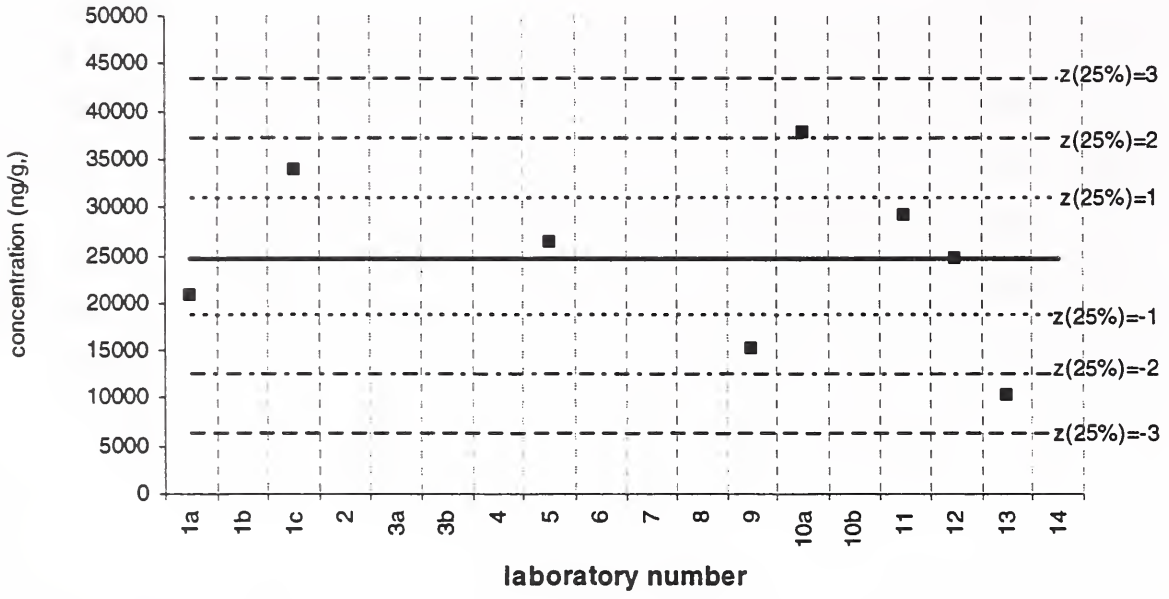


n-C28

SRM 1648

Assigned value (solid line) = 24762 ng/g s = 9224 ng/g 95% CL = 7712 ng/g

Reported Results: 8 Quantitative Results: 8

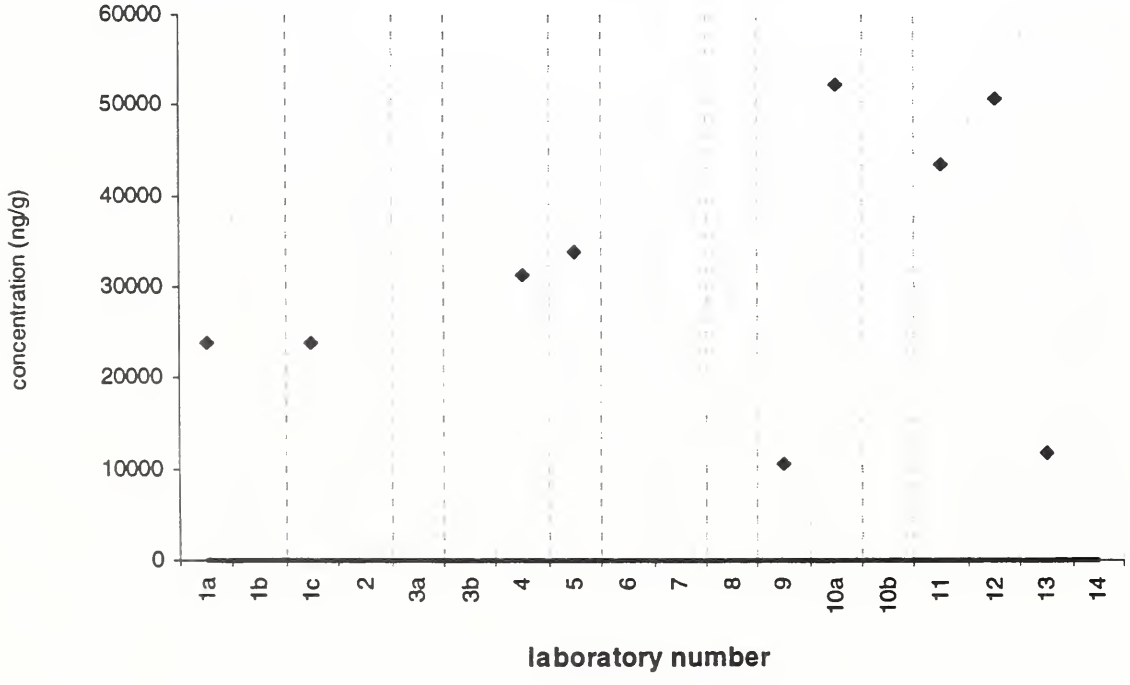


n-C28

SRM 1649a

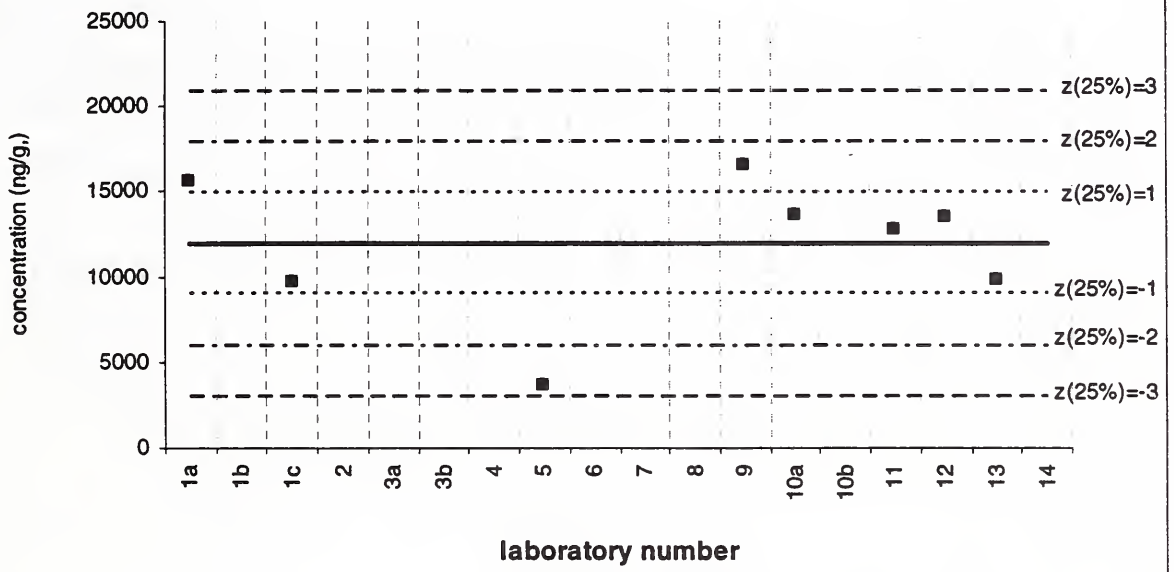
Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9



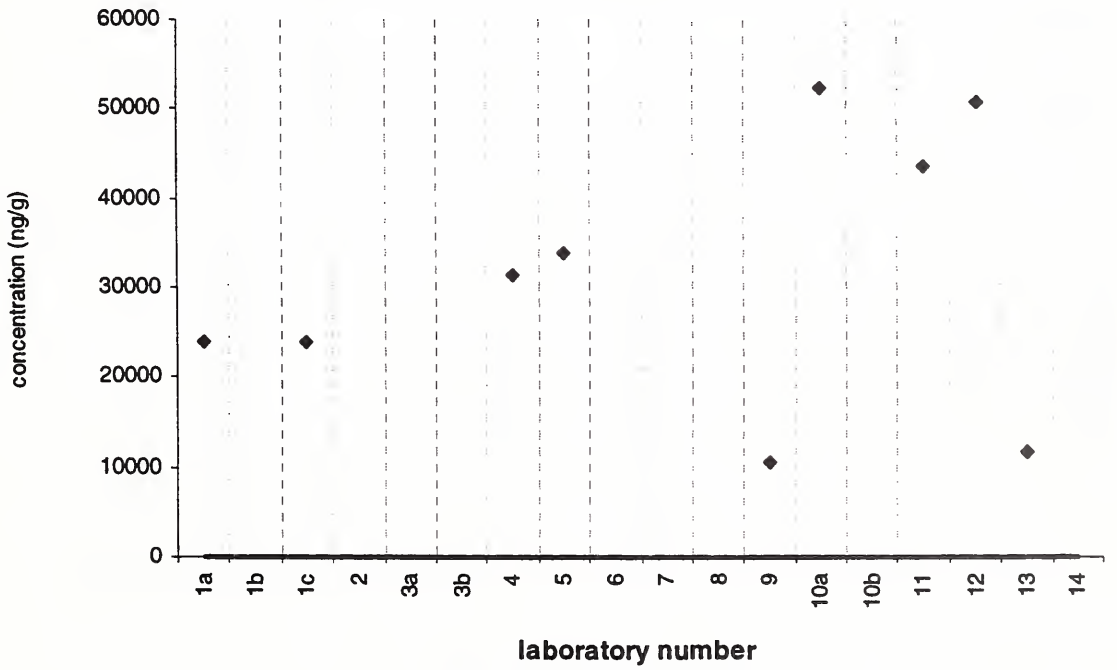
n-C28 Baltimore 2 PM

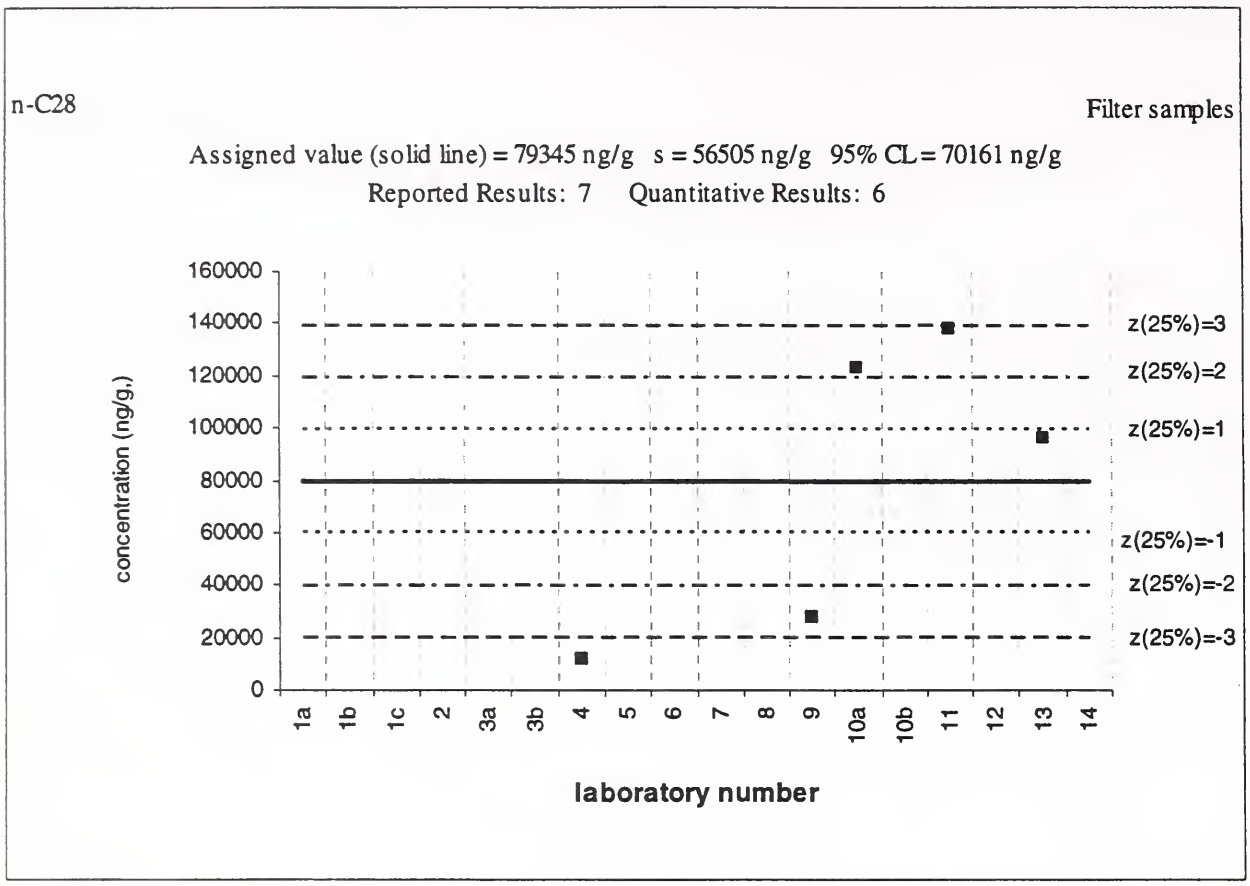
Assigned value (solid line) = 11930 ng/g s = 4139 ng/g 95% CL = 3460 ng/g
Reported Results: 8 Quantitative Results: 8



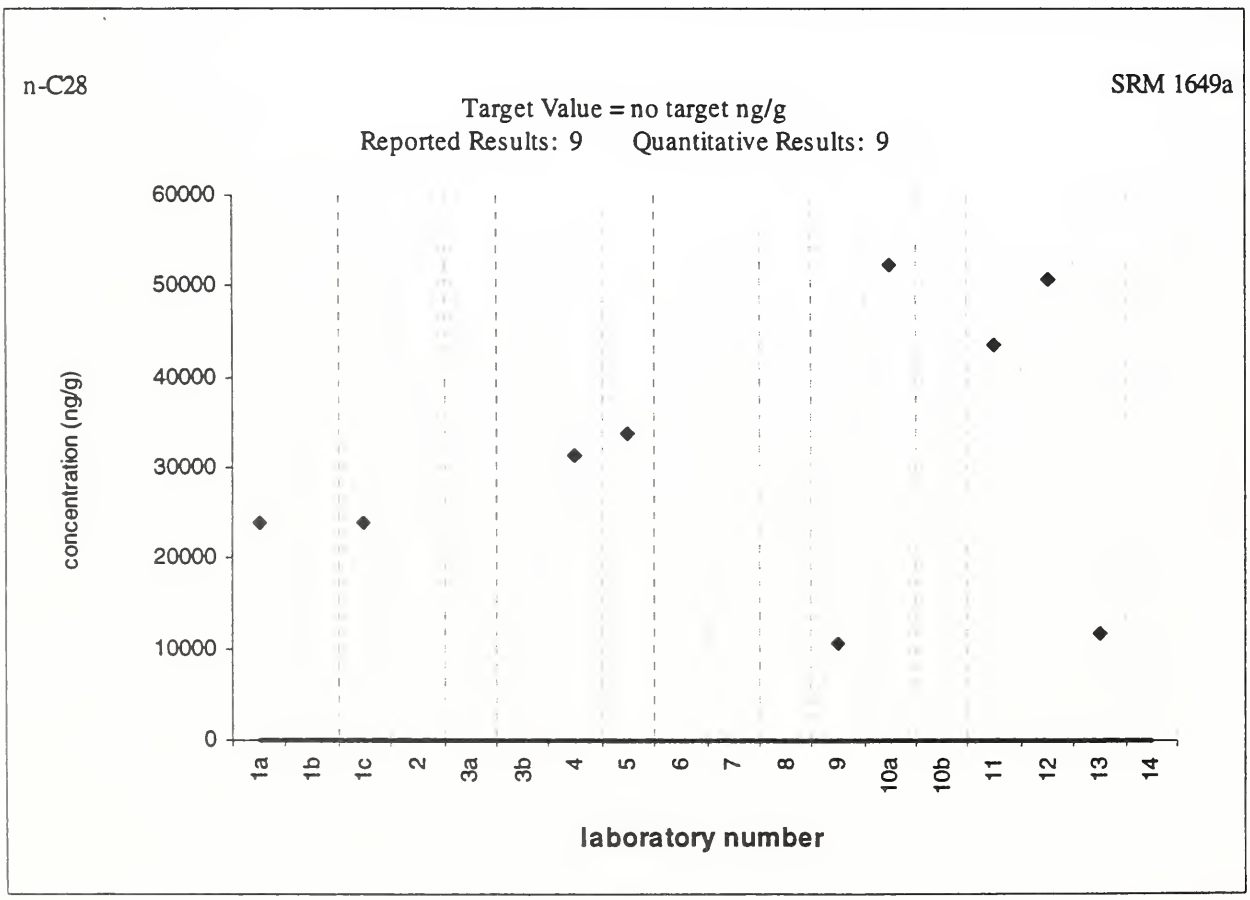
n-C28 SRM 1649a

Target Value = no target ng/g
Reported Results: 9 Quantitative Results: 9





lab 12 = 309752 ng/g

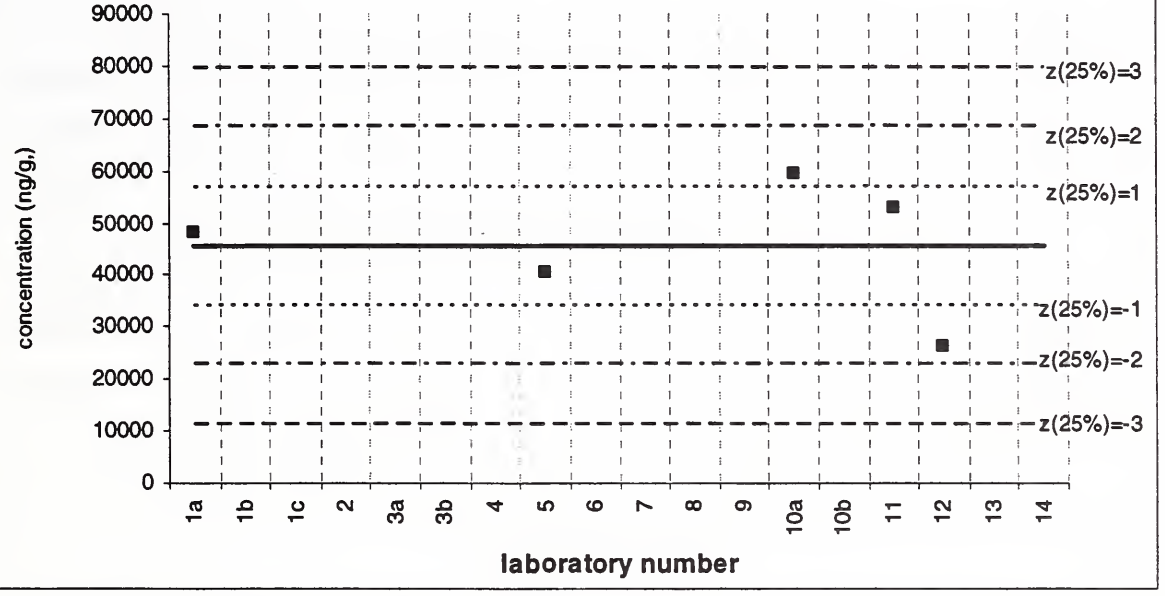


n-C29

SRM 1648

Assigned value (solid line) = 45541 ng/g s = 12885 ng/g 95% CL = 15999 ng/g

Reported Results: 5 Quantitative Results: 5

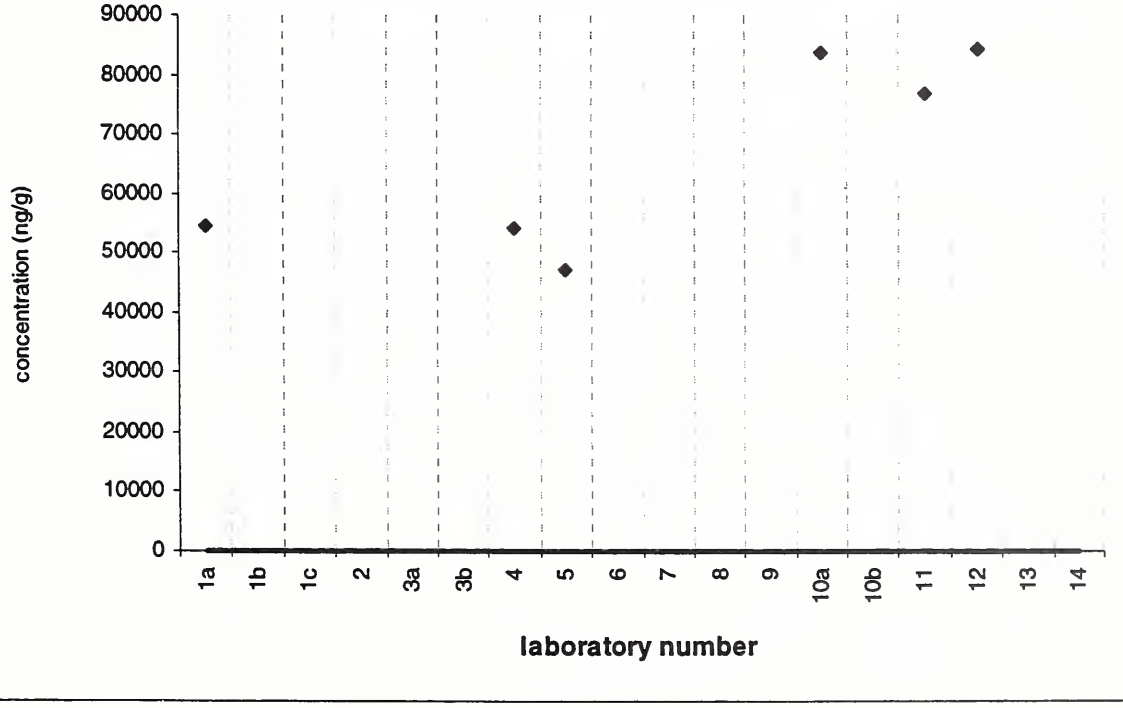


n-C29

SRM 1649a

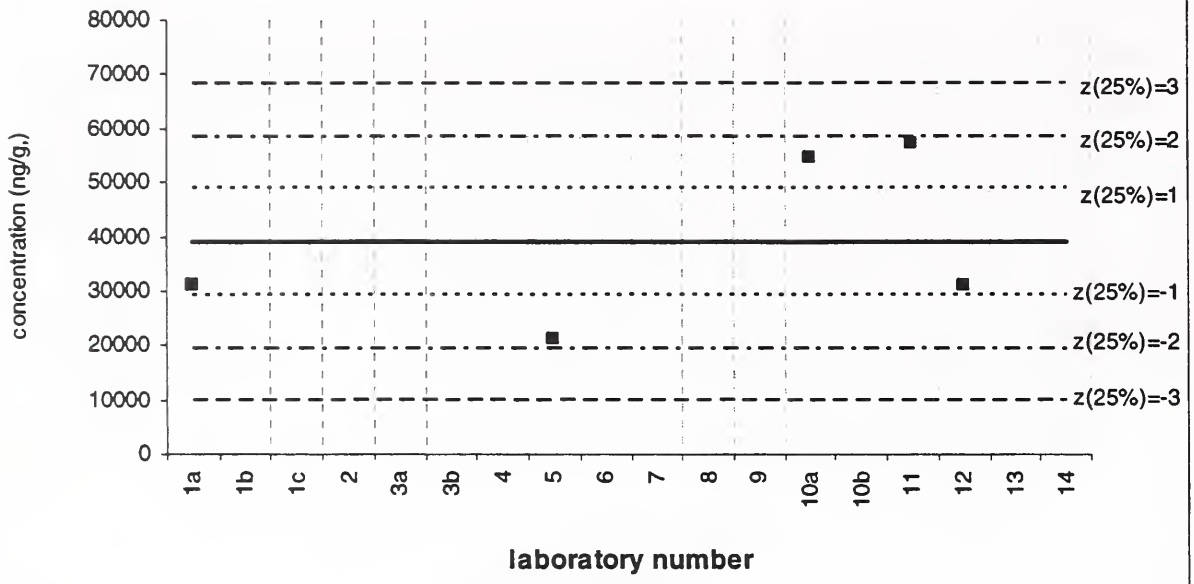
Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6



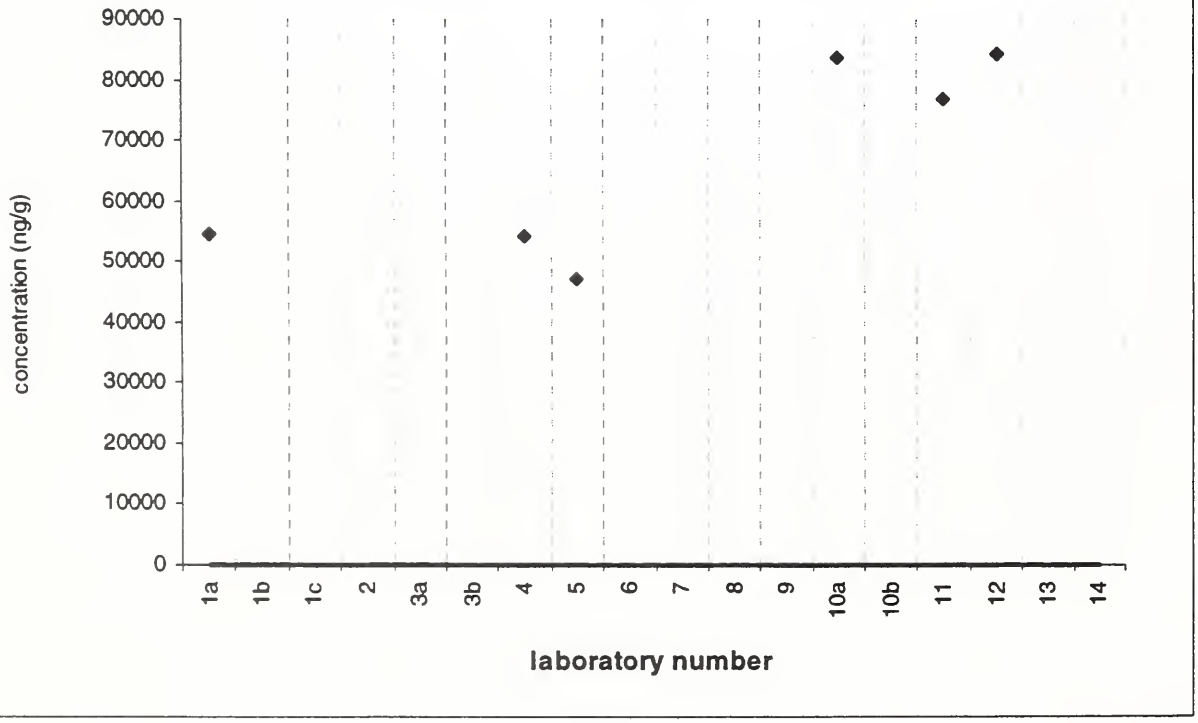
n-C29 Baltimore 2 PM

Assigned value (solid line) = 39039 ng/g s = 16028 ng/g 95% CL = 19901 ng/g
Reported Results: 5 Quantitative Results: 5



n-C29 SRM 1649a

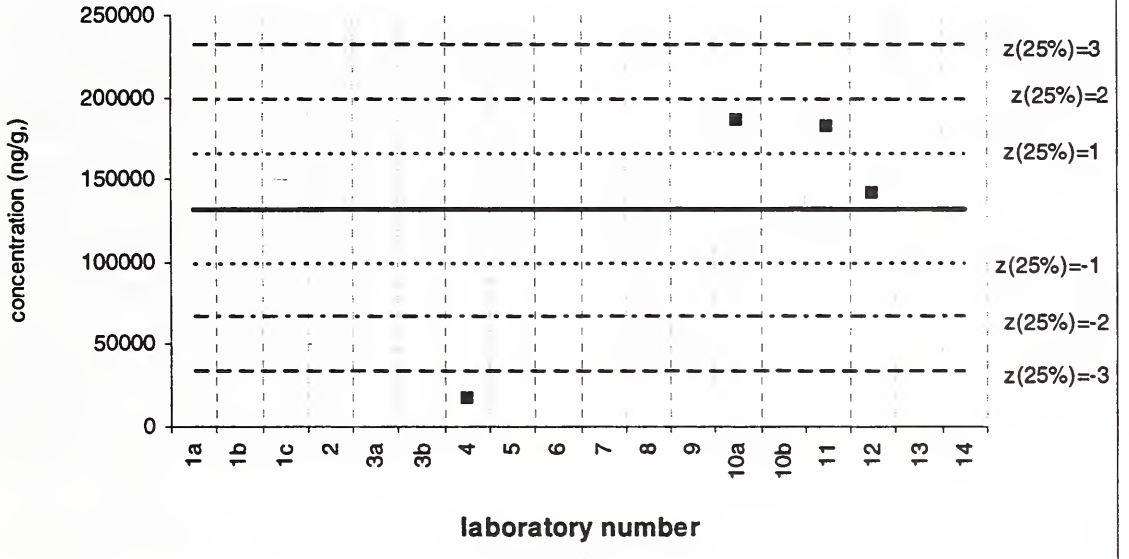
Target Value = no target ng/g
Reported Results: 6 Quantitative Results: 6



n-C29 Filter samples

Assigned value (solid line) = 131999 ng/g s = 78746 ng/g 95% CL = 125303 ng/g

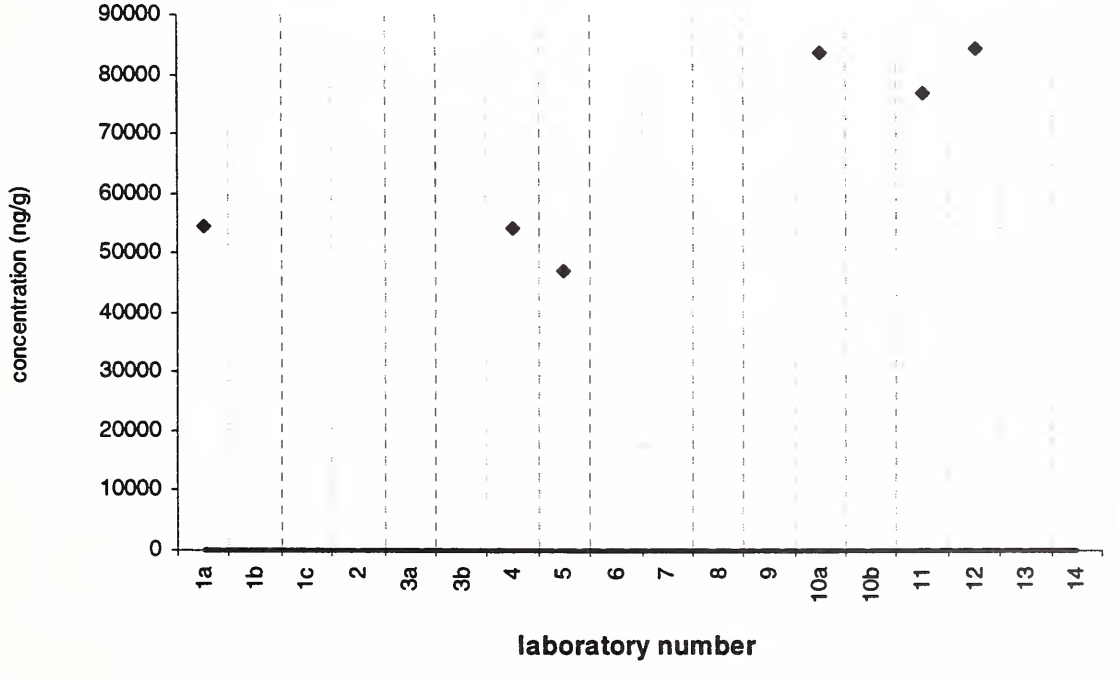
Reported Results: 4 Quantitative Results: 4



n-C29 SRM 1649a

Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6

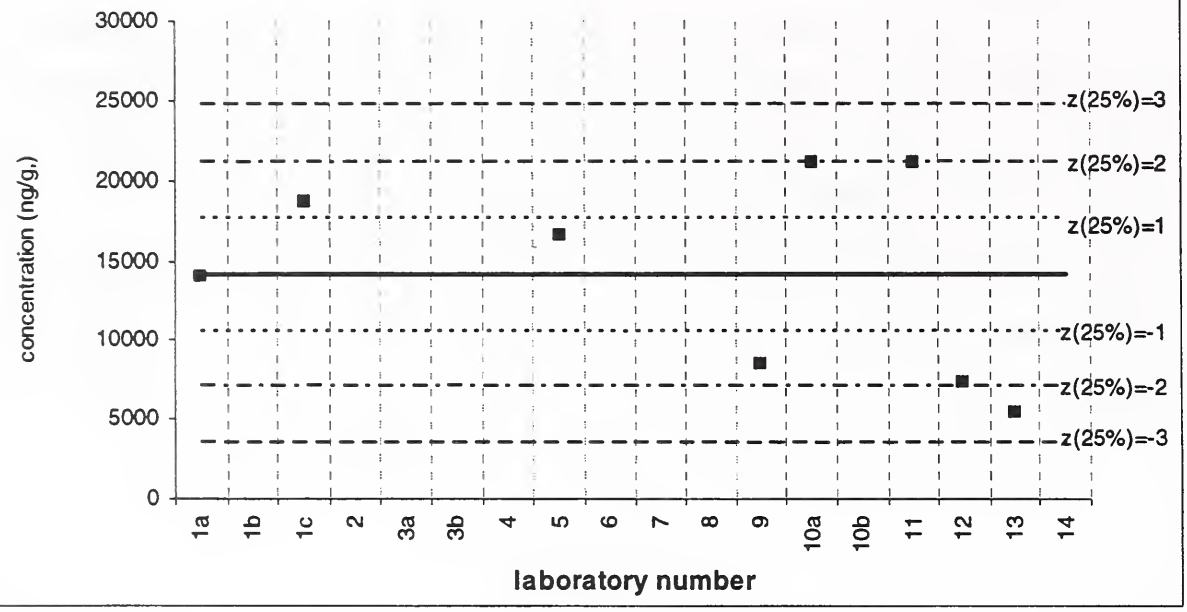


n-C30

SRM 1648

Assigned value (solid line) = 14102 ng/g s = 6320 ng/g 95% CL = 5283 ng/g

Reported Results: 8 Quantitative Results: 8

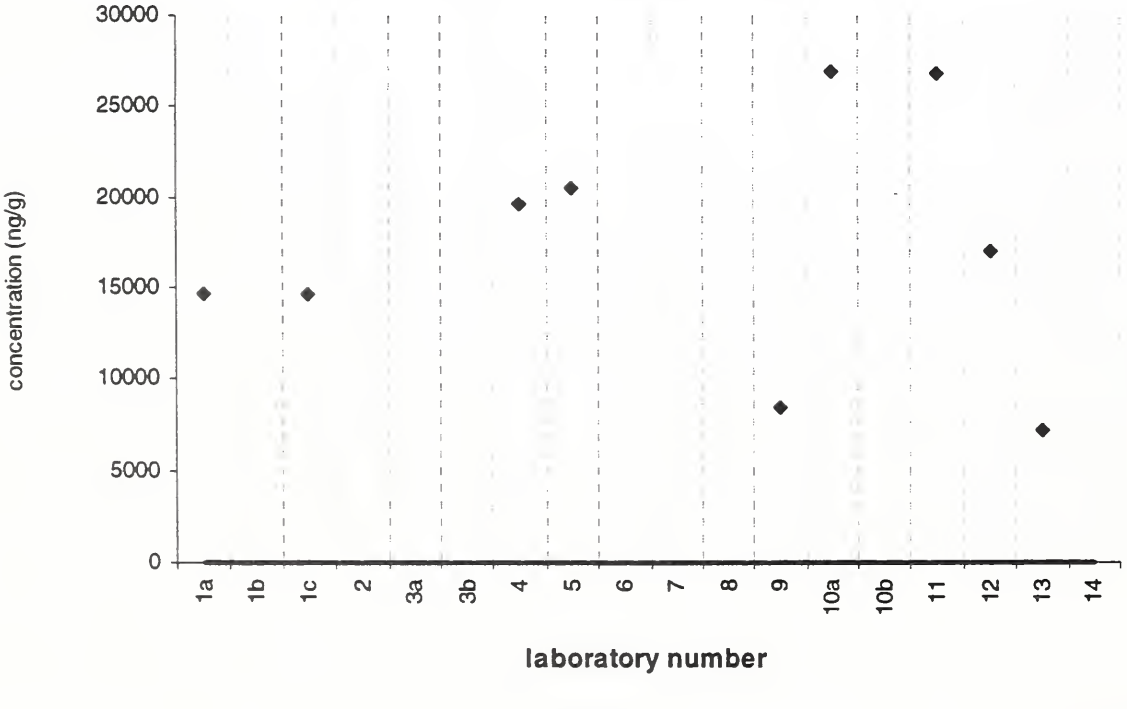


n-C30

SRM 1649a

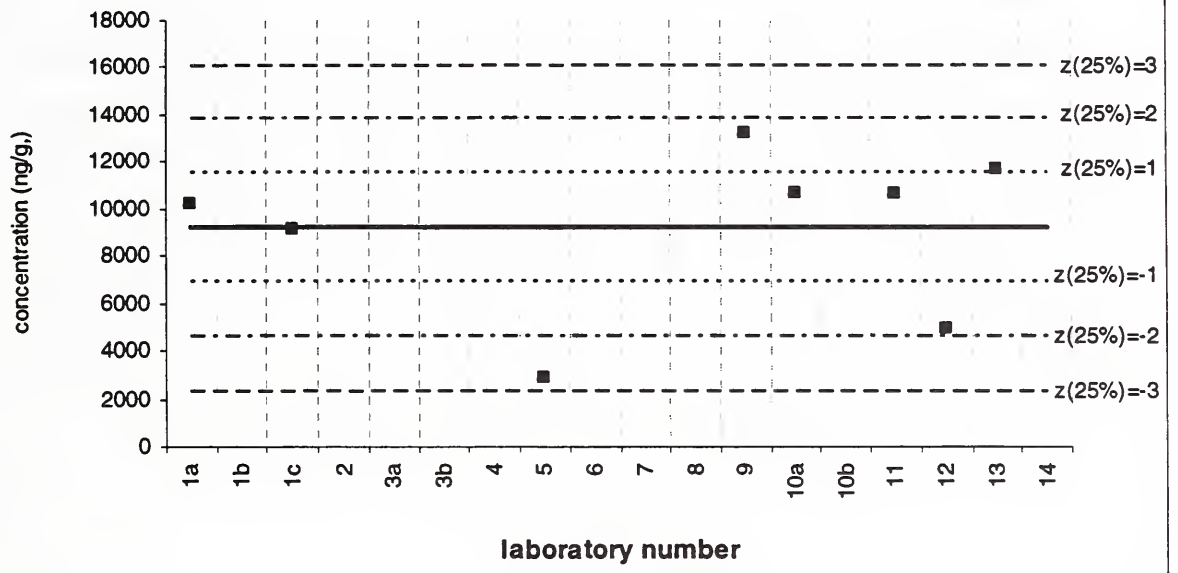
Target Value = no target ng/g

Reported Results: 9 Quantitative Results: 9



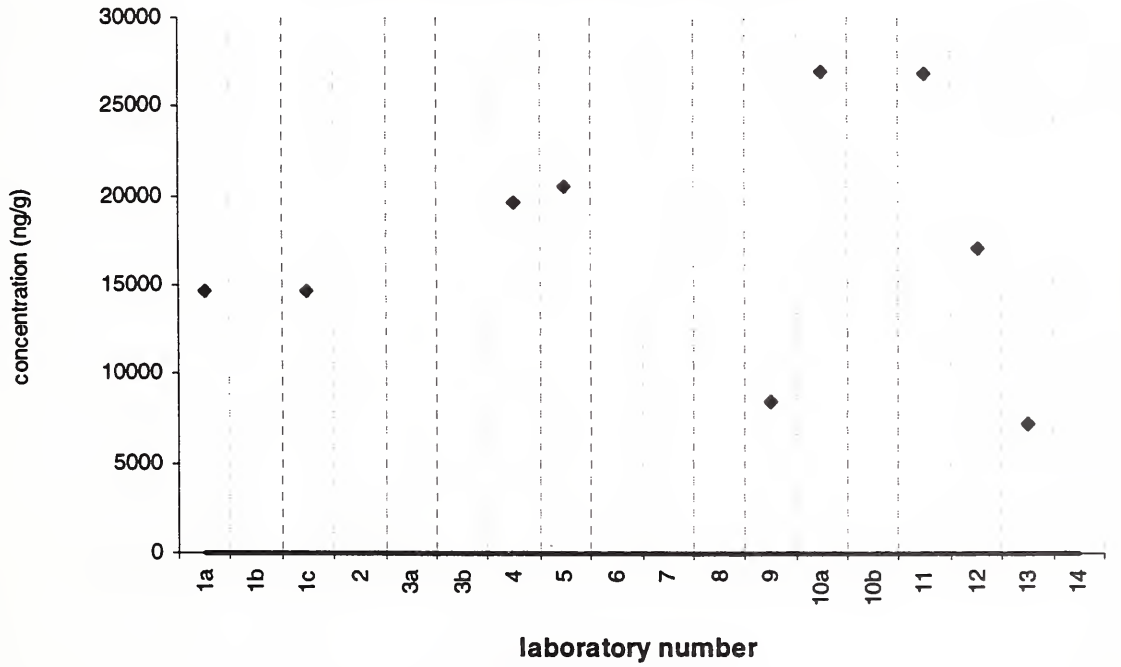
n-C30 Baltimore 2 PM

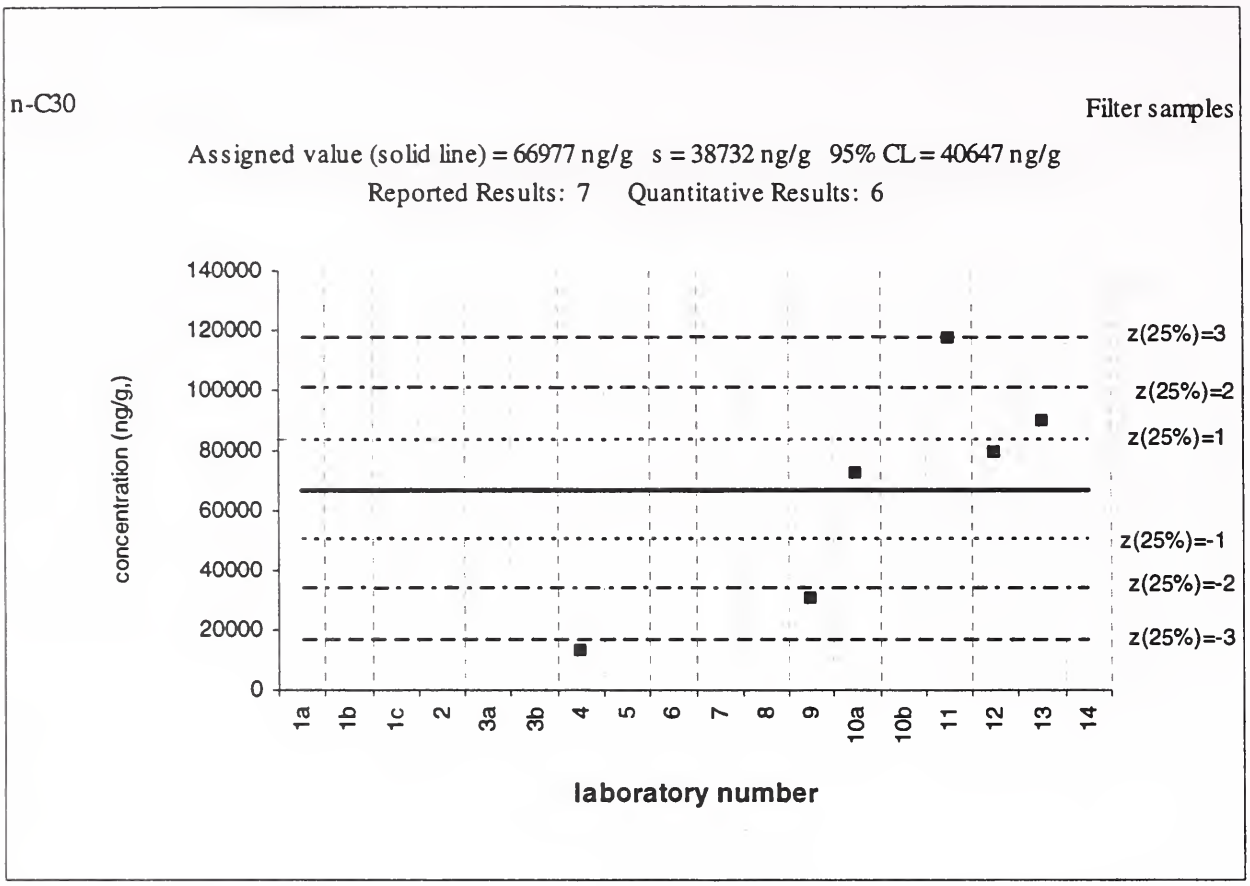
Assigned value (solid line) = 9187 ng/g s = 3486 ng/g 95% CL = 2914 ng/g
Reported Results: 8 Quantitative Results: 8

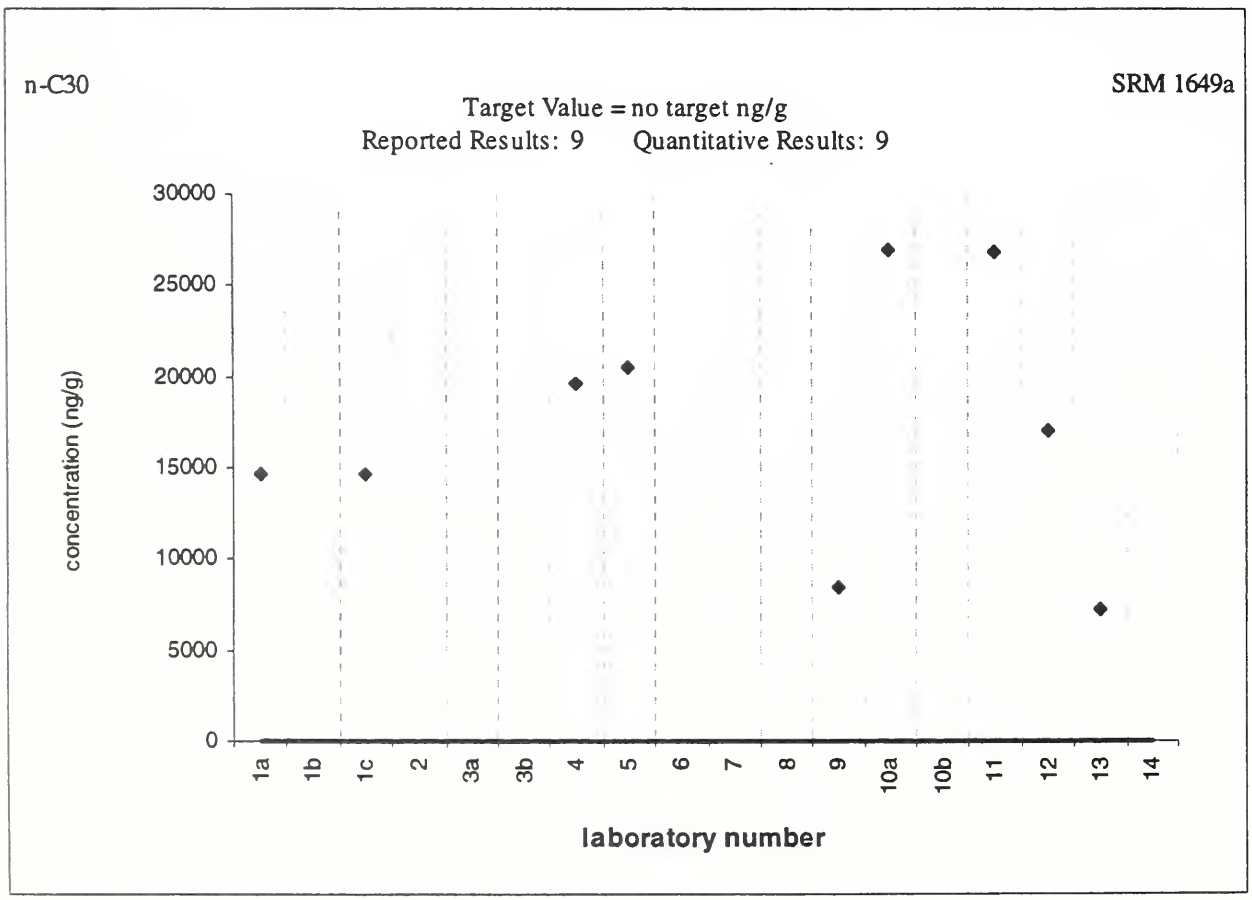


n-C30 SRM 1649a

Target Value = no target ng/g
Reported Results: 9 Quantitative Results: 9




n-C30
Filter samples
Assigned value (solid line) = 66977 ng/g s = 38732 ng/g 95% CL = 40647 ng/g
Reported Results: 7 Quantitative Results: 6
concentration (ng/g)
140000
120000
100000
80000
60000
40000
20000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

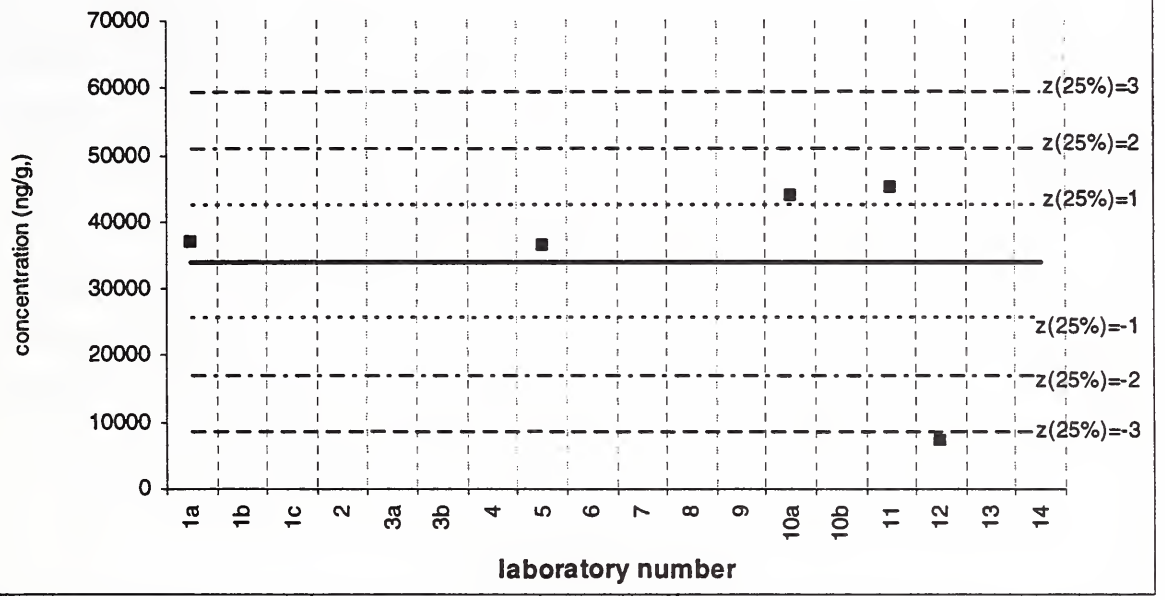

n-C30
SRM 1649a
Target Value = no target ng/g
Reported Results: 9 Quantitative Results: 9
concentration (ng/g)
30000
25000
20000
15000
10000
5000
0
1a 1b 1c 2 3a 3b 4 5 6 7 8 9 10a 10b 11 12 13 14
laboratory number

n-C31

SRM 1648

Assigned value (solid line) = 33870 ng/g s = 15345 ng/g 95% CL = 19054 ng/g

Reported Results: 5 Quantitative Results: 5

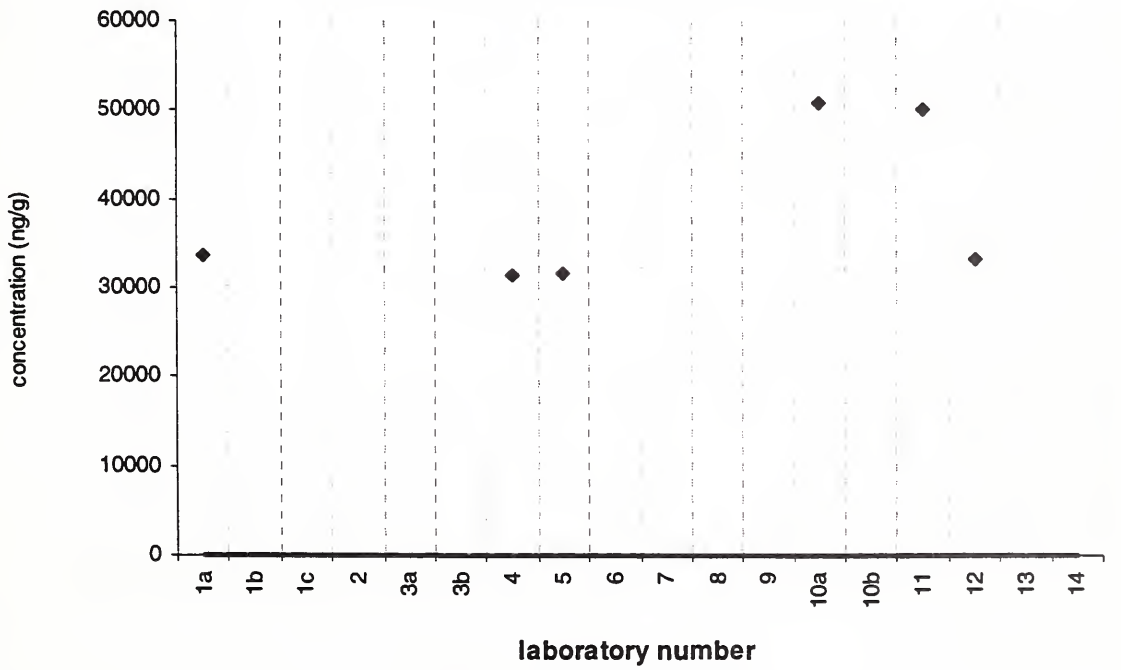


n-C31

SRM 1649a

Target Value = no target ng/g

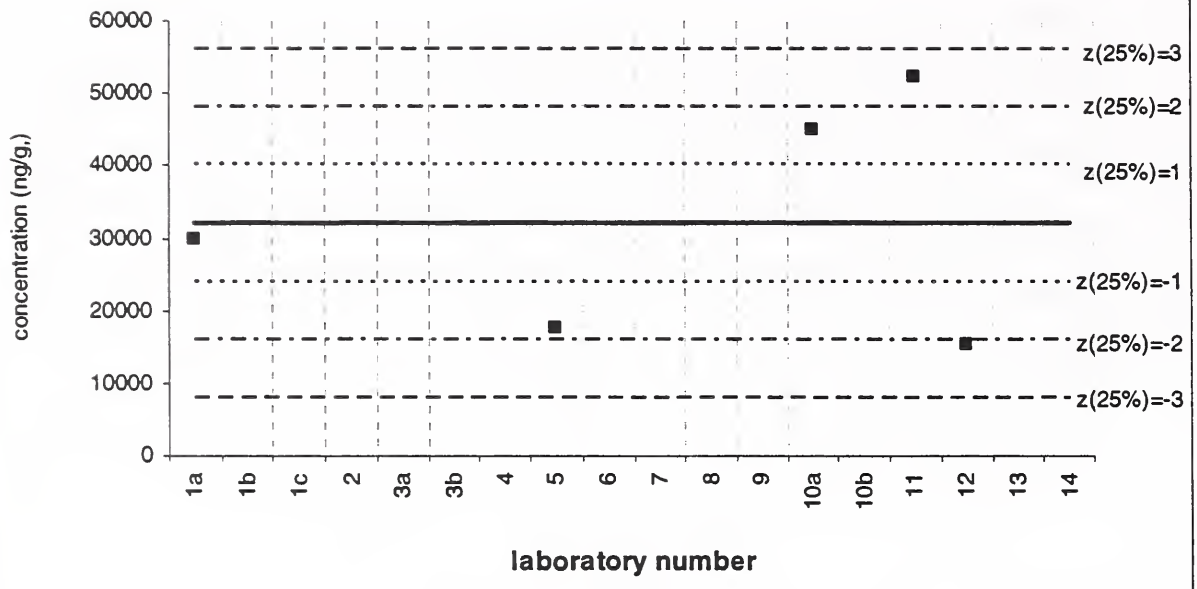
Reported Results: 6 Quantitative Results: 6



n-C31 Baltimore 2 PM

Assigned value (solid line) = 32007 ng/g s = 16344 ng/g 95% CL = 20294 ng/g

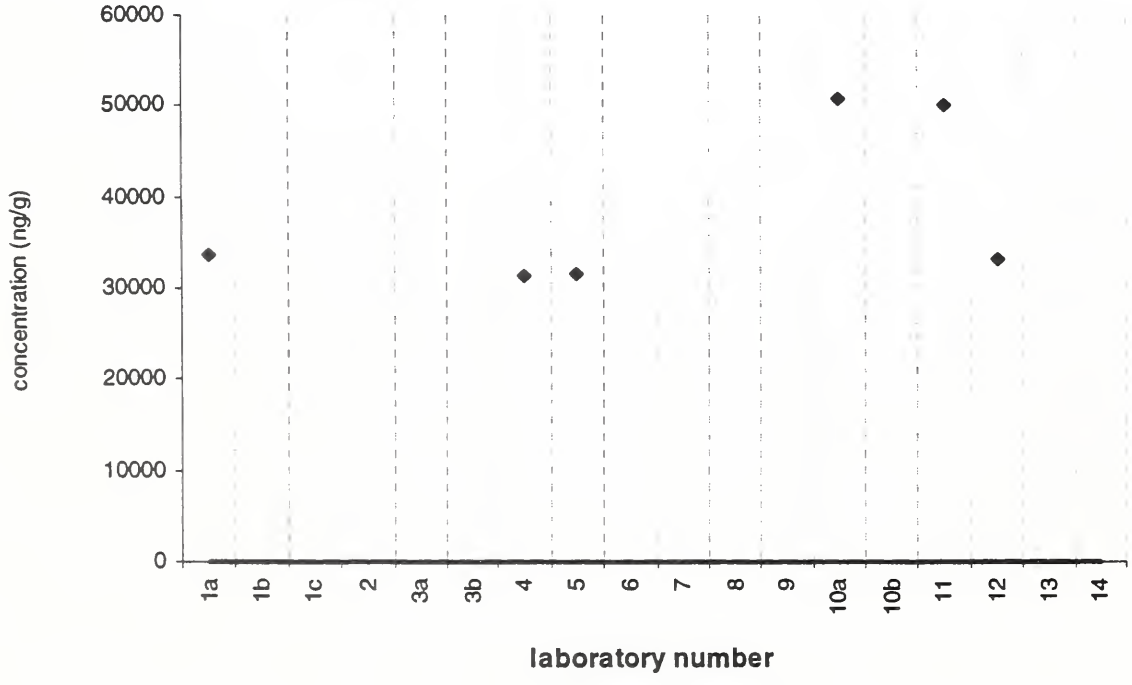
Reported Results: 5 Quantitative Results: 5



n-C31 SRM 1649a

Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6

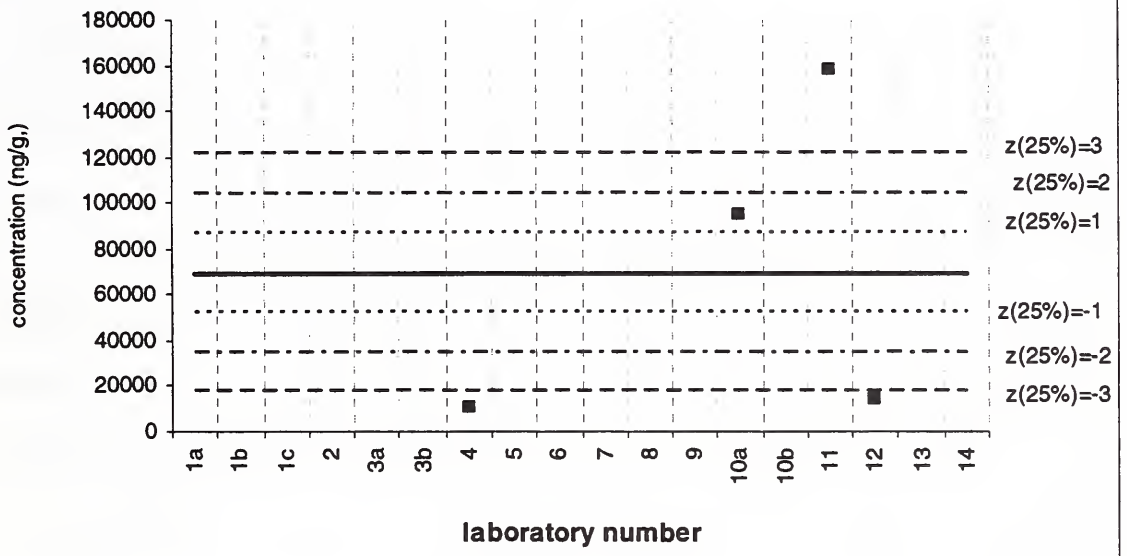


n-C31

Filter samples

Assigned value (solid line) = 69239 ng/g s = 70863 ng/g 95% CL = 112760 ng/g

Reported Results: 4 Quantitative Results: 4

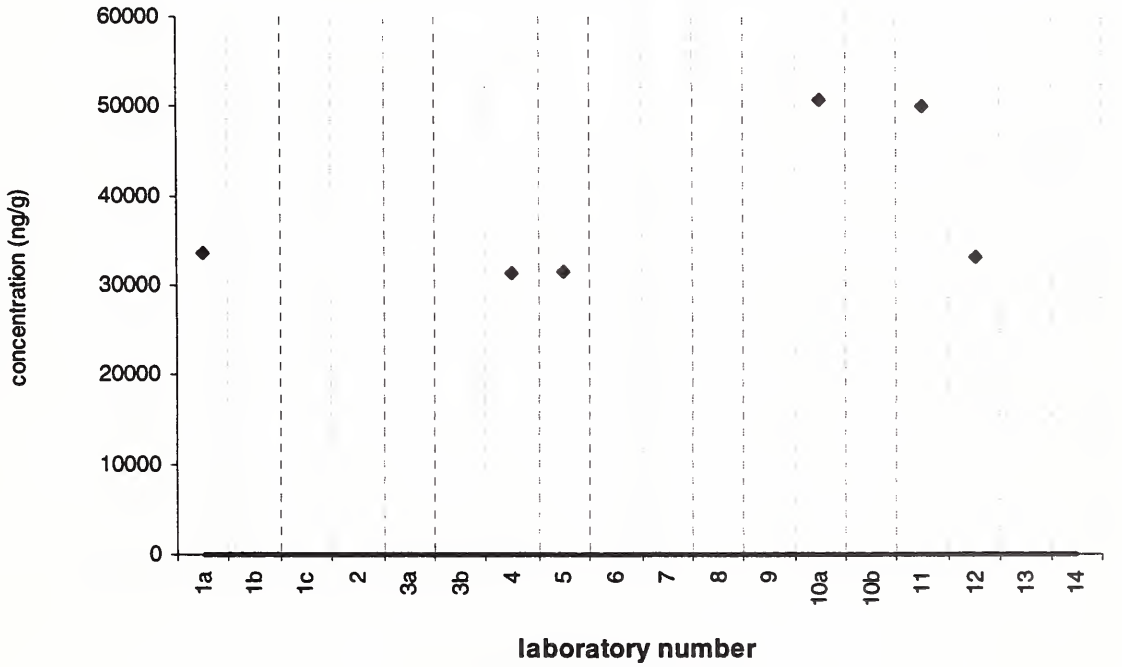


n-C31

SRM 1649a

Target Value = no target ng/g

Reported Results: 6 Quantitative Results: 6

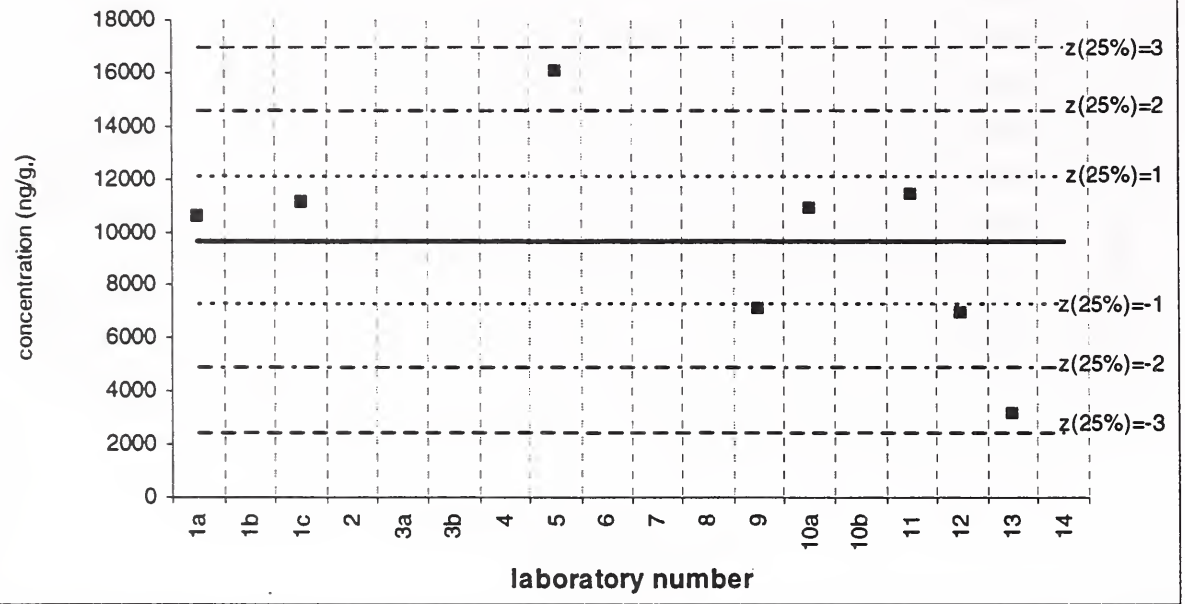


n-C32

SRM 1648

Assigned value (solid line) = 9669 ng/g s = 3855 ng/g 95% CL = 3222 ng/g

Reported Results: 8 Quantitative Results: 8

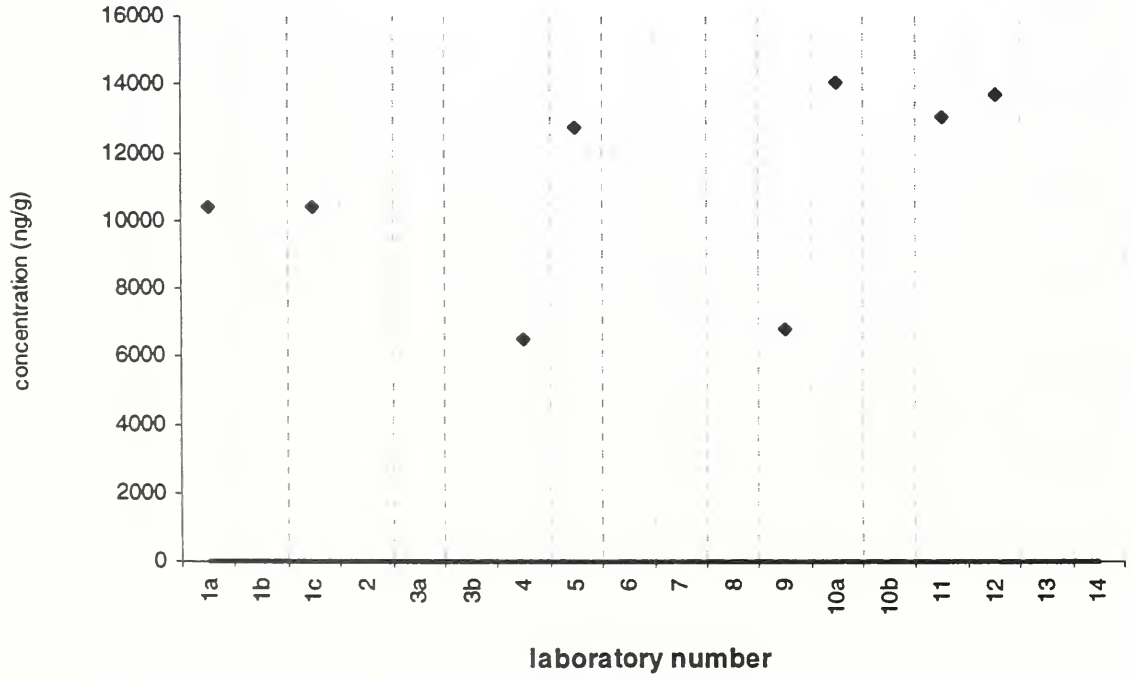


n-C32

SRM 1649a

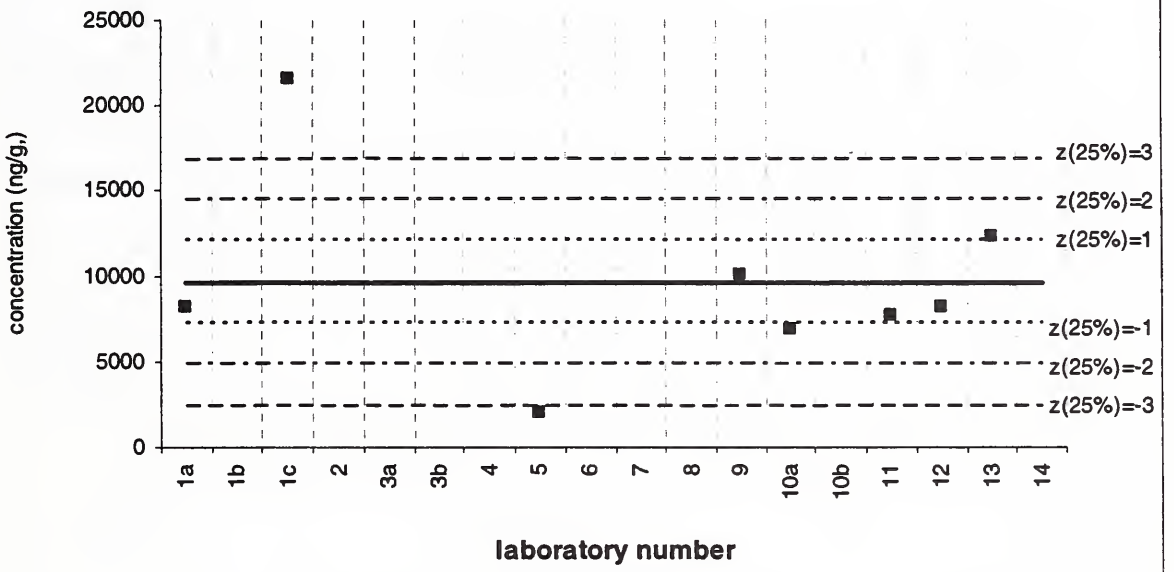
Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 8



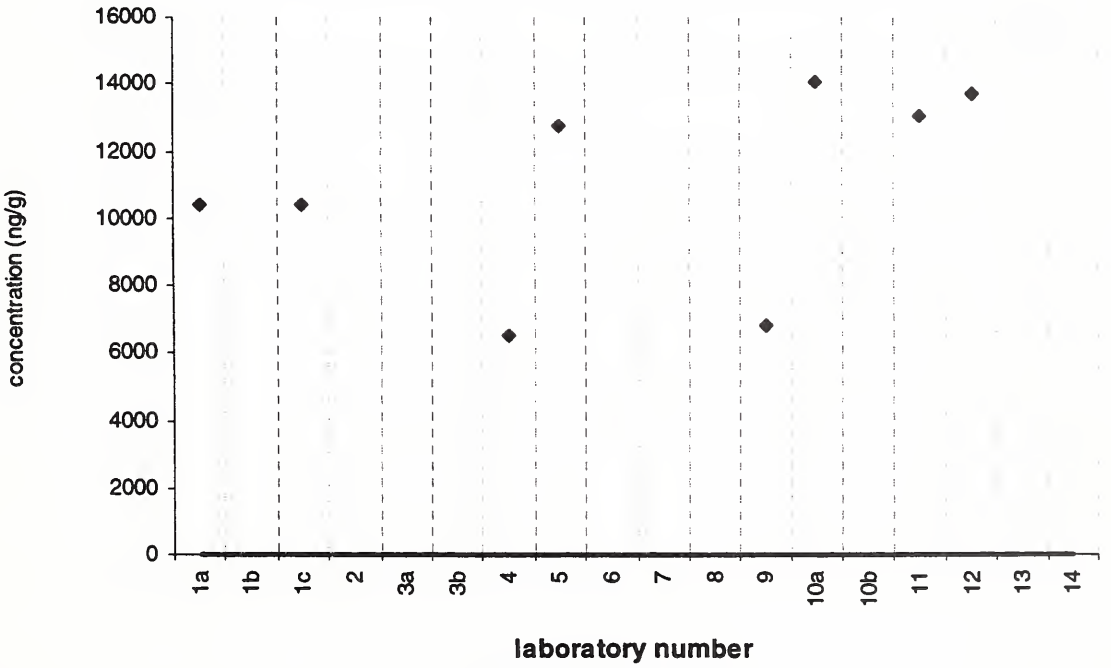
n-C32 Baltimore 2 PM

Assigned value (solid line) = 9625 ng/g s = 5650 ng/g 95% CL = 4723 ng/g
Reported Results: 8 Quantitative Results: 8



n-C32 SRM 1649a

Target Value = no target ng/g
Reported Results: 8 Quantitative Results: 8

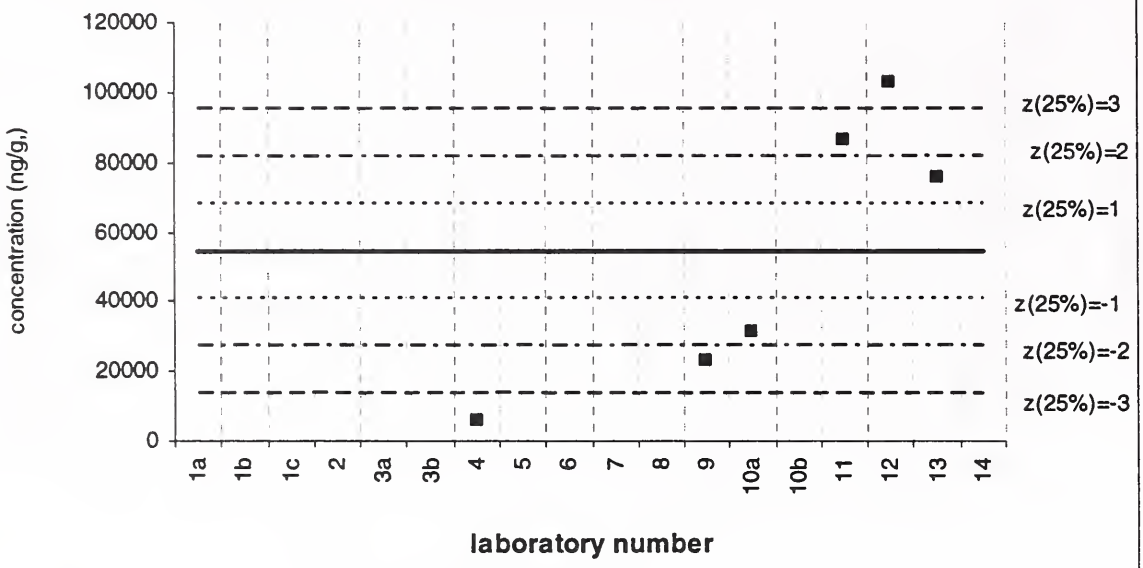


n-C32

Filter samples

Assigned value (solid line) = 54312 ng/g s = 39255 ng/g 95% CL = 41195 ng/g

Reported Results: 7 Quantitative Results: 6



n-C32

SRM 1649a

Target Value = no target ng/g

Reported Results: 8 Quantitative Results: 8

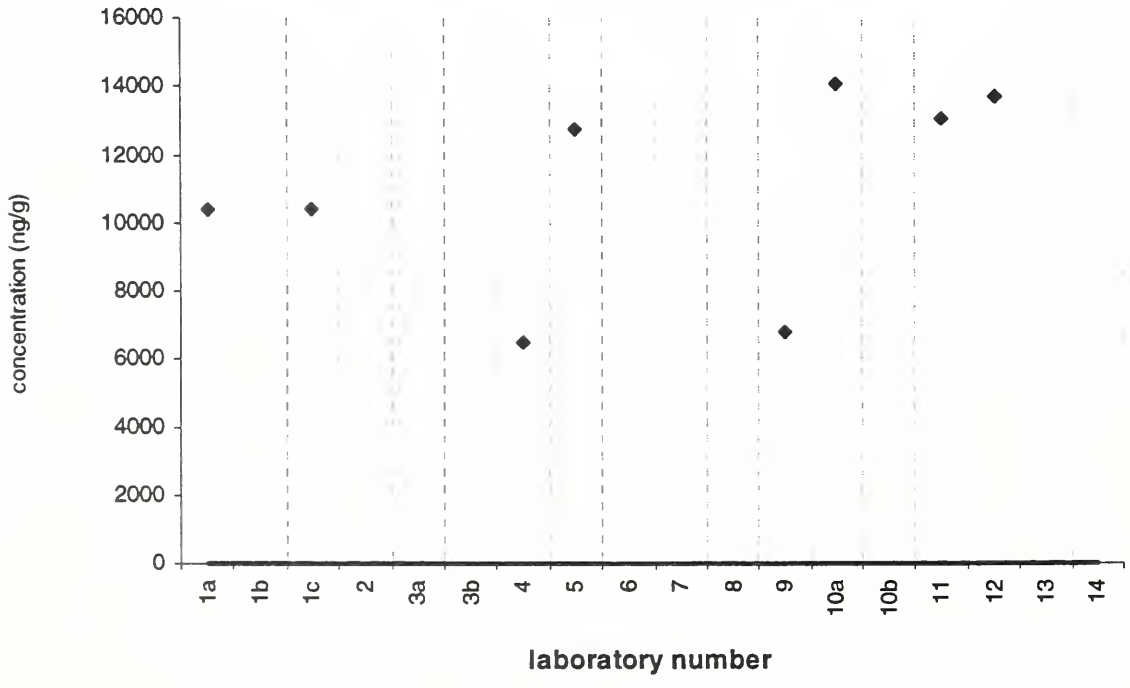


abb 20R Cholestane (Chiron#0602,27)

SRM 1648

Assigned value (solid line) = 1413 ng/g s = 100 ng/g 95% CL = 898 ng/g

Reported Results: 2 Quantitative Results: 2

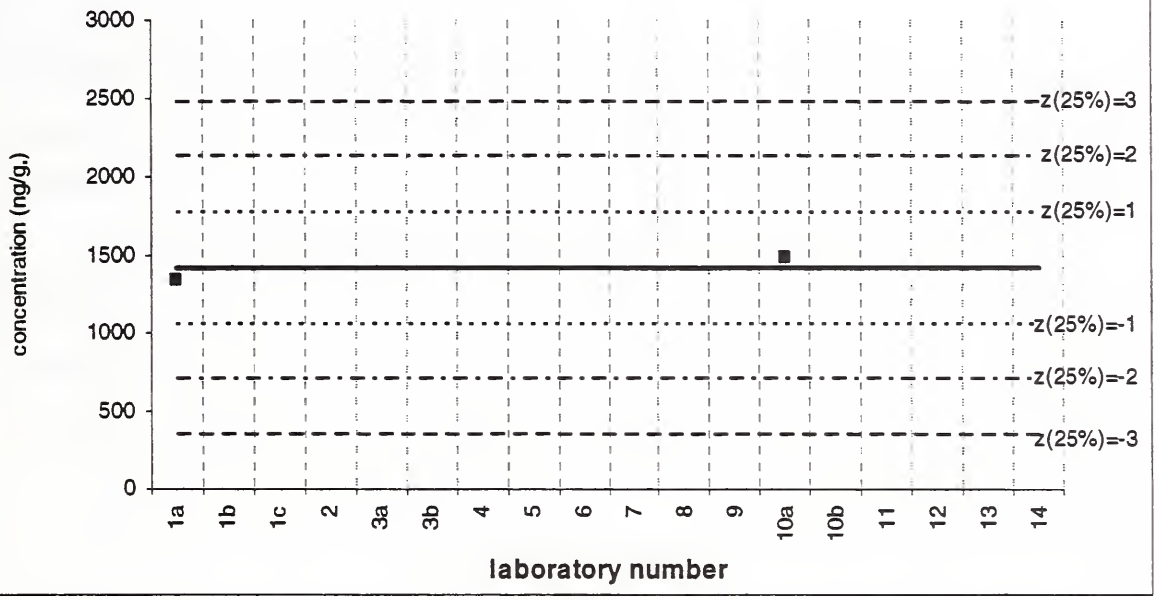
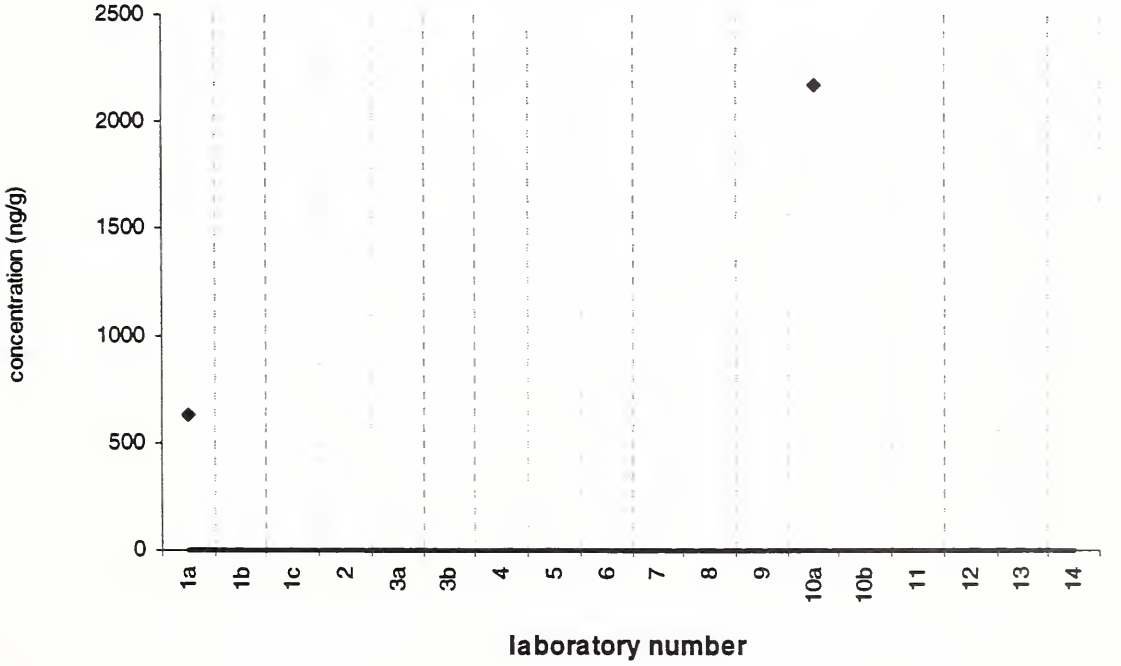


abb 20R Cholestane (Chiron#0602,27)

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

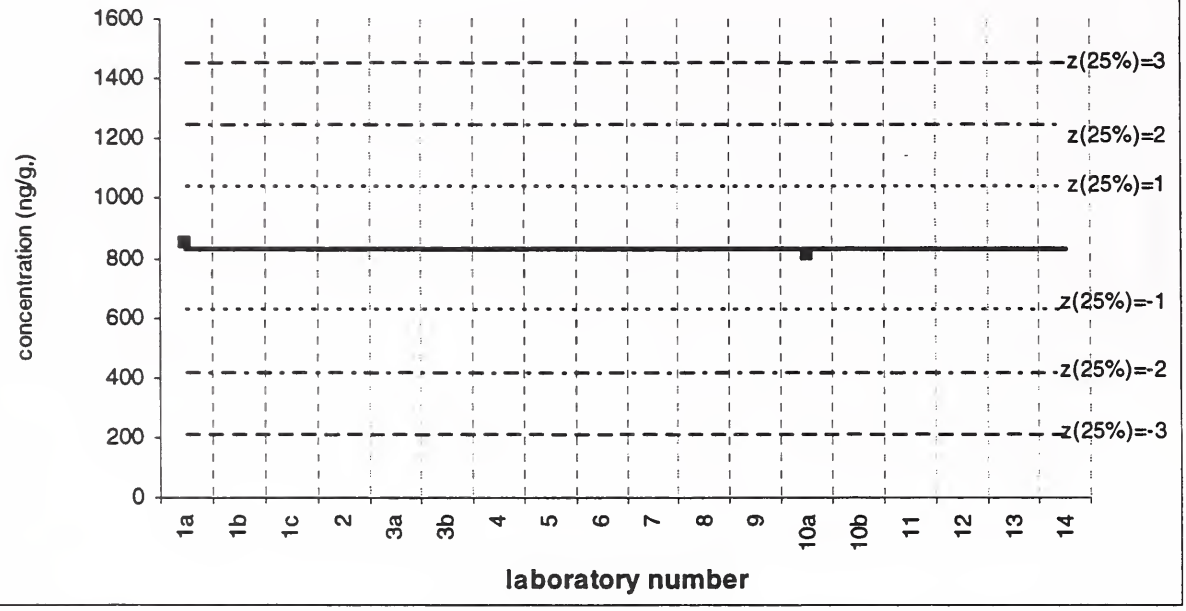


aaa 20R-Cholestane (Chiron#0622,27)

SRM 1648

Assigned value (solid line) = 830 ng/g s = 32 ng/g 95% CL = 288 ng/g

Reported Results: 2 Quantitative Results: 2

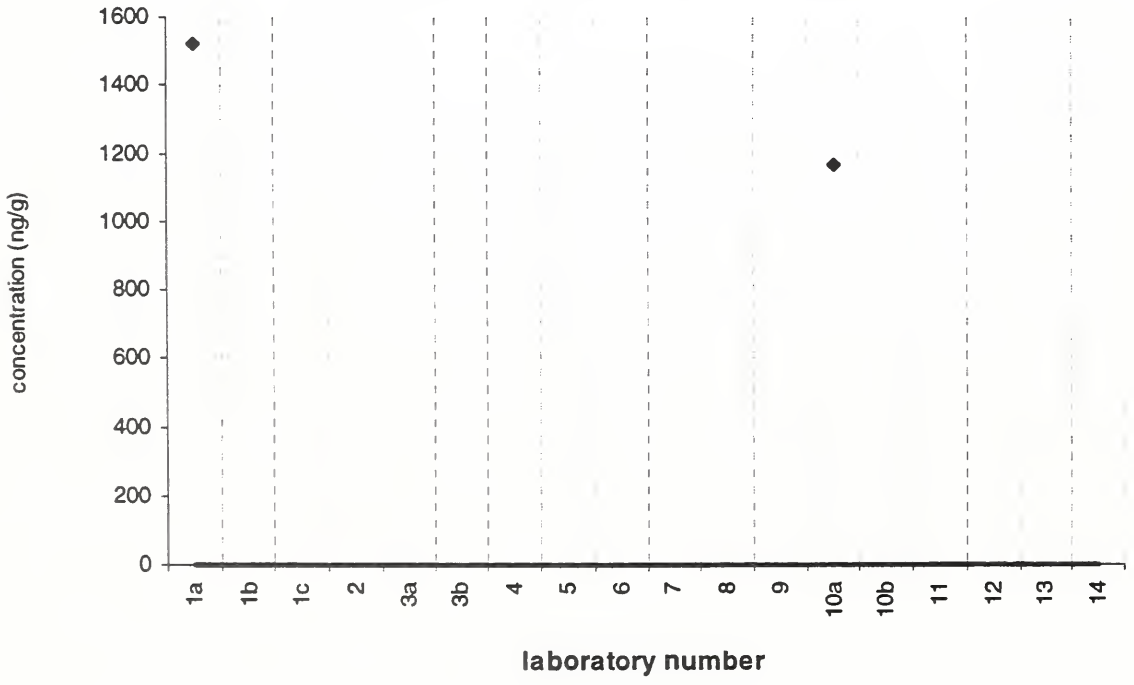


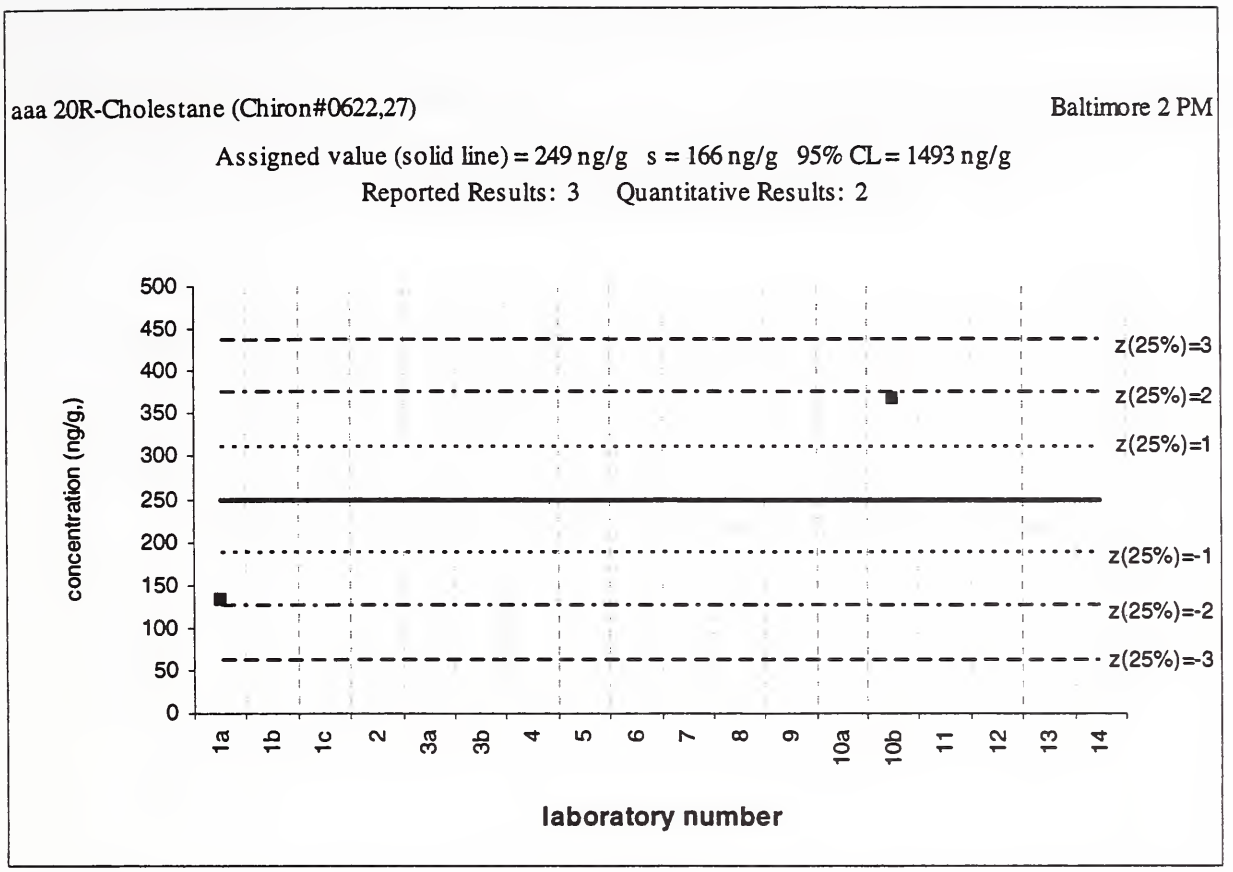
aaa 20R-Cholestane (Chiron#0622,27)

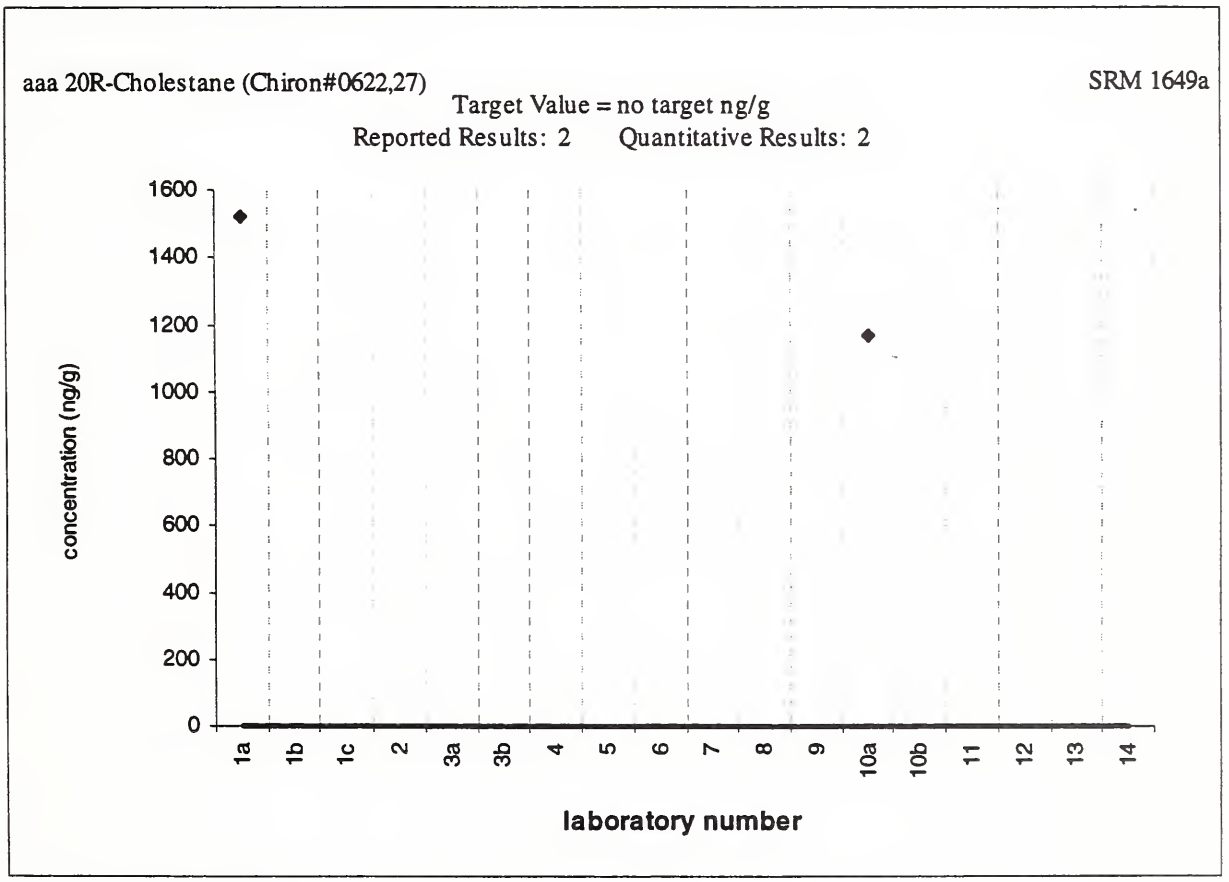
SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2




aaa 20R-Cholestane (Chiron#0622,27)
Baltimore 2 PM
Assigned value (solid line) = 249 ng/g s = 166 ng/g 95% CL = 1493 ng/g
Reported Results: 3 Quantitative Results: 2
concentration (ng/g,)
500
450
400
350
300
250
200
150
100
50
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

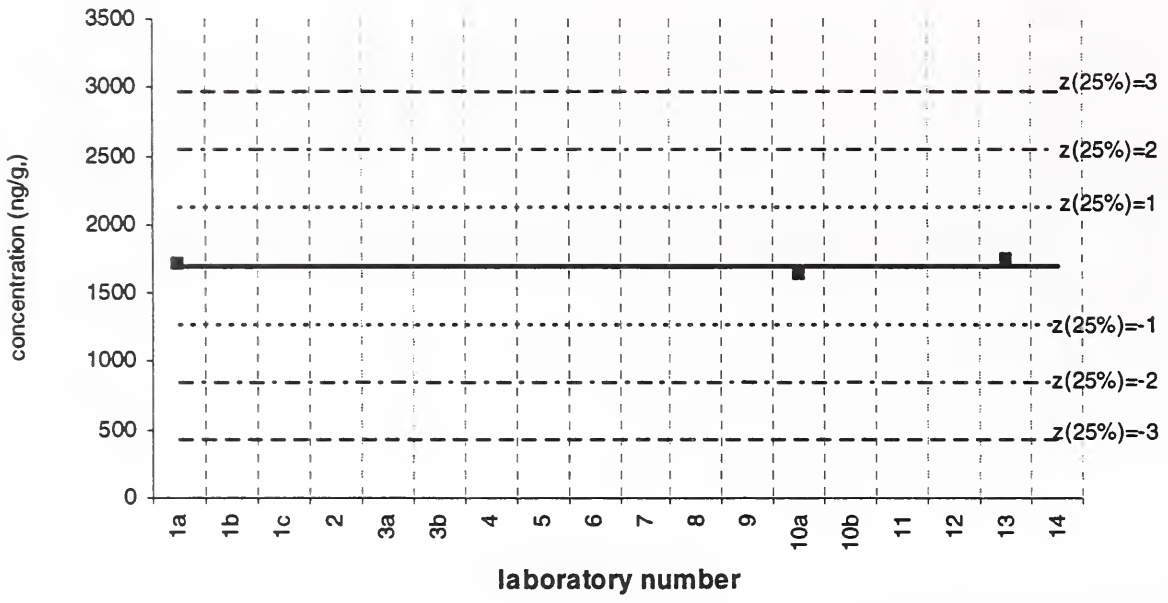

aaa 20R-Cholestane (Chiron#0622,27)
SRM 1649a
Target Value = no target ng/g
Reported Results: 2 Quantitative Results: 2
concentration (ng/g)
1600
1400
1200
1000
800
600
400
200
0
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)

SRM 1648

Assigned value (solid line) = 1692 ng/g s = 55 ng/g 95% CL = 137 ng/g

Reported Results: 4 Quantitative Results: 3

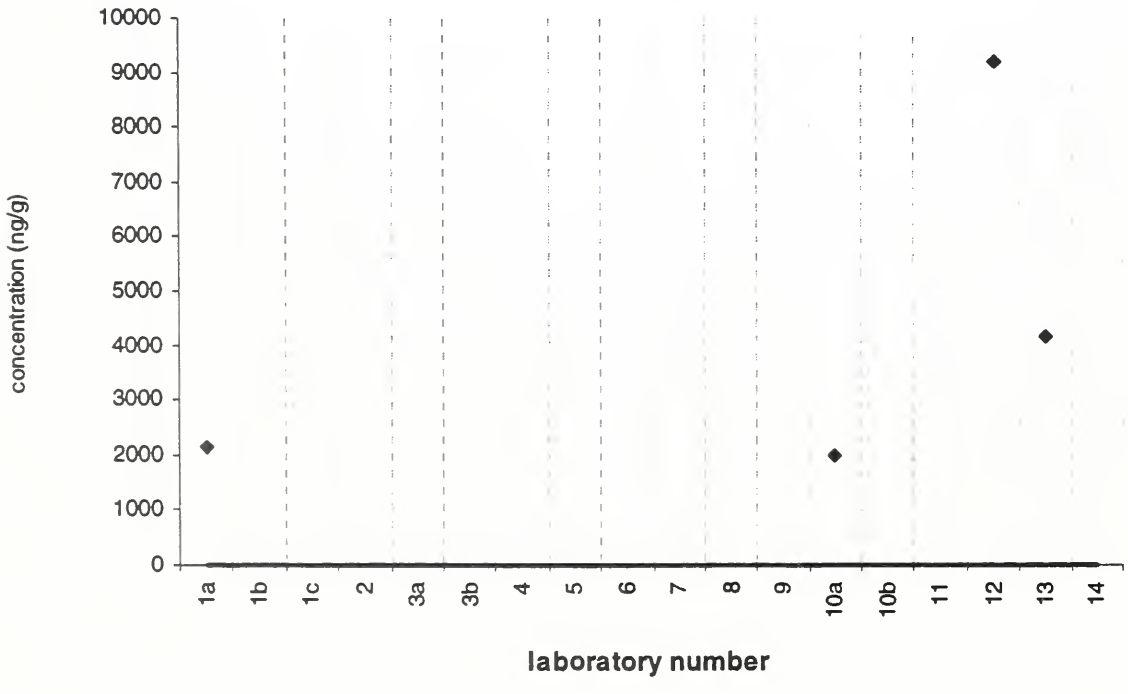


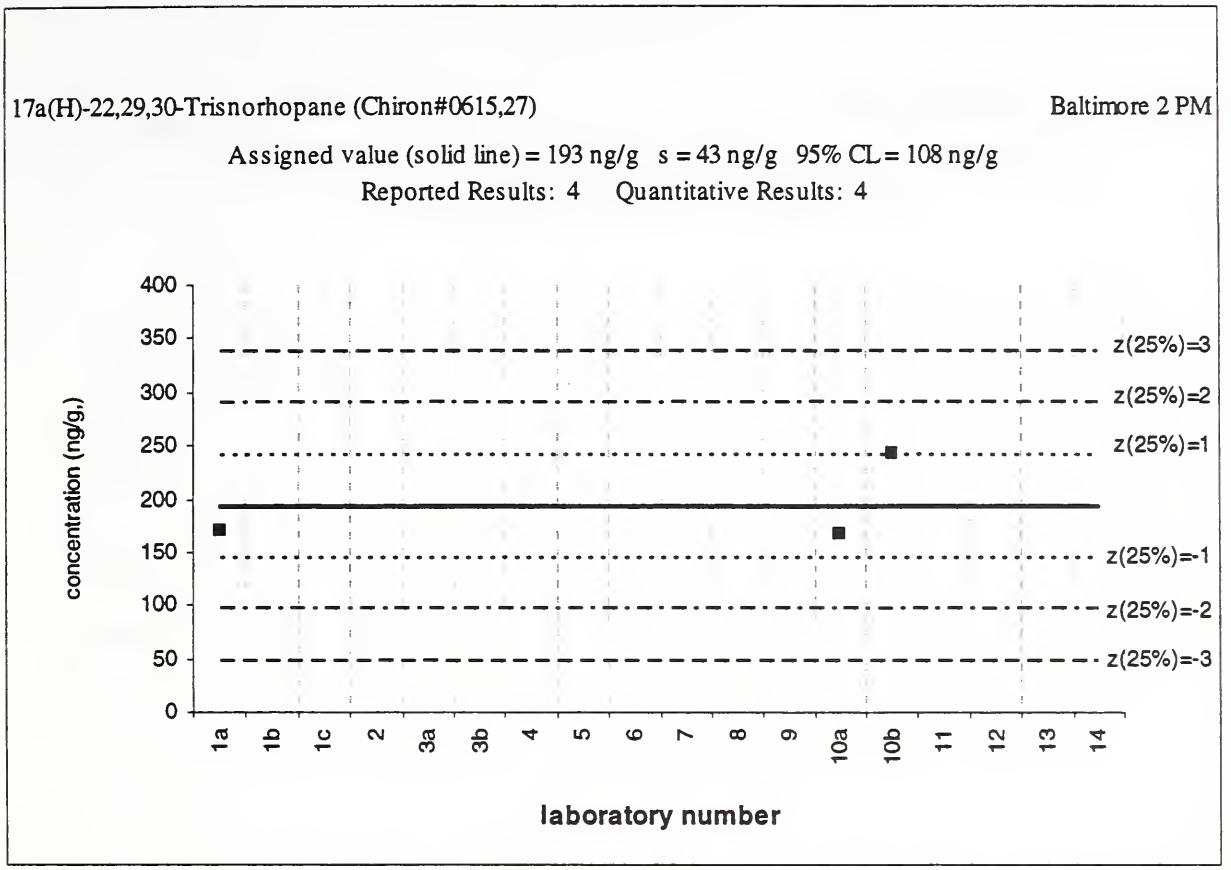
17a(H)-22,29,30-Trisnorhopane (Chiron#0615,27)

SRM 1649a

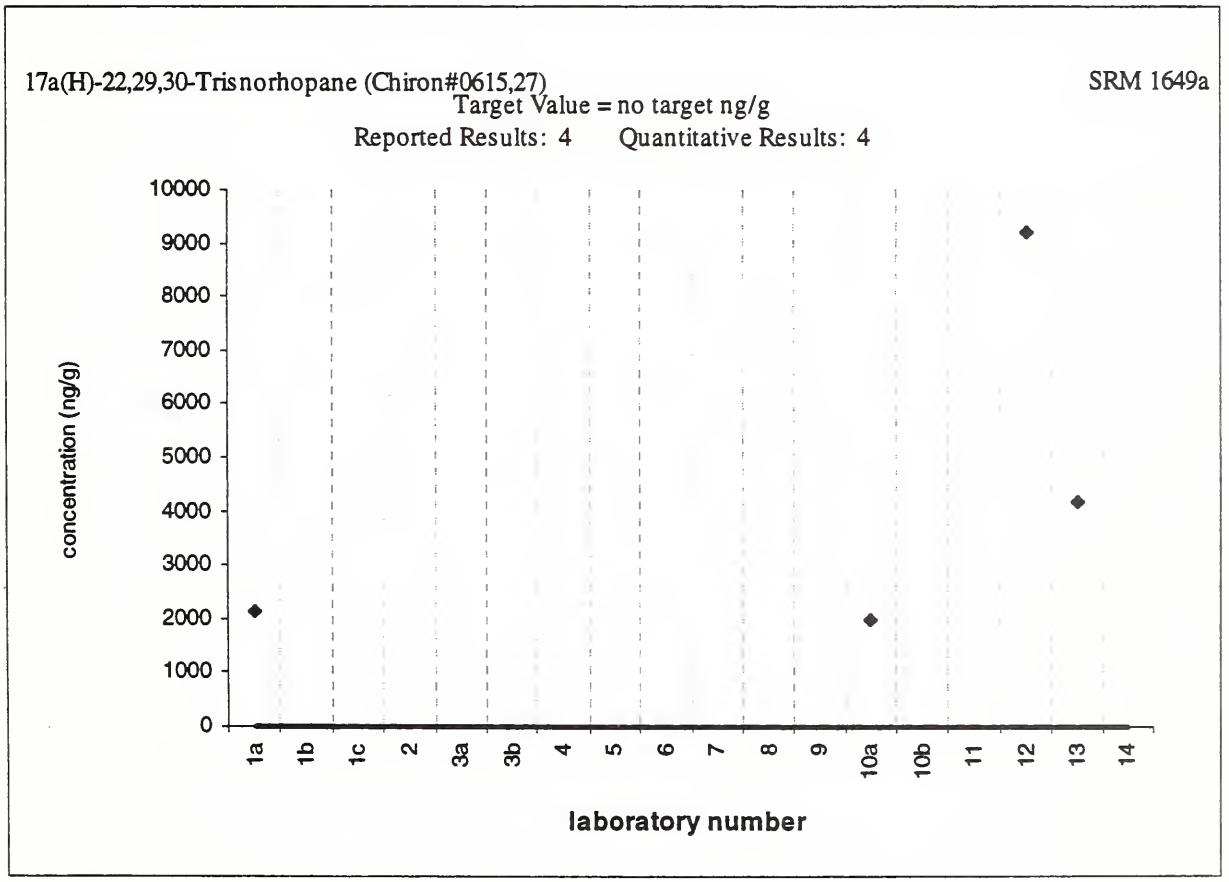
Target Value = no target ng/g

Reported Results: 4 Quantitative Results: 4





lab 12 = 16735 ng/g

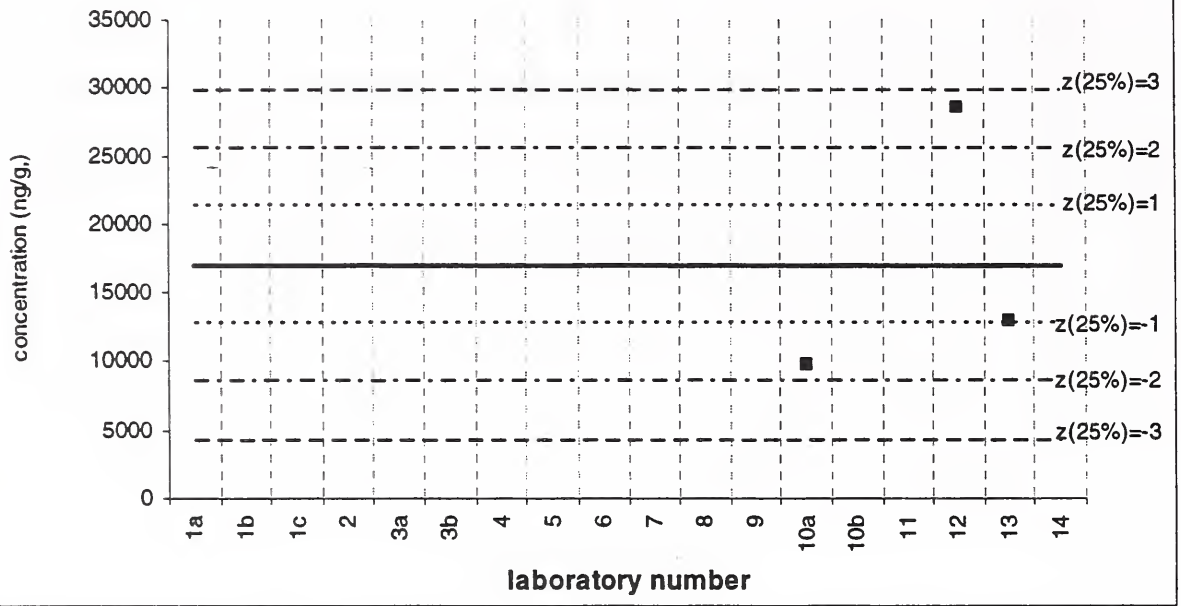


17a(H),21b(H)-Hopane (Chiron#0132,30)

SRM 1648

Assigned value (solid line) = 17037 ng/g s = 10059 ng/g 95% CL = 24989 ng/g

Reported Results: 3 Quantitative Results: 3

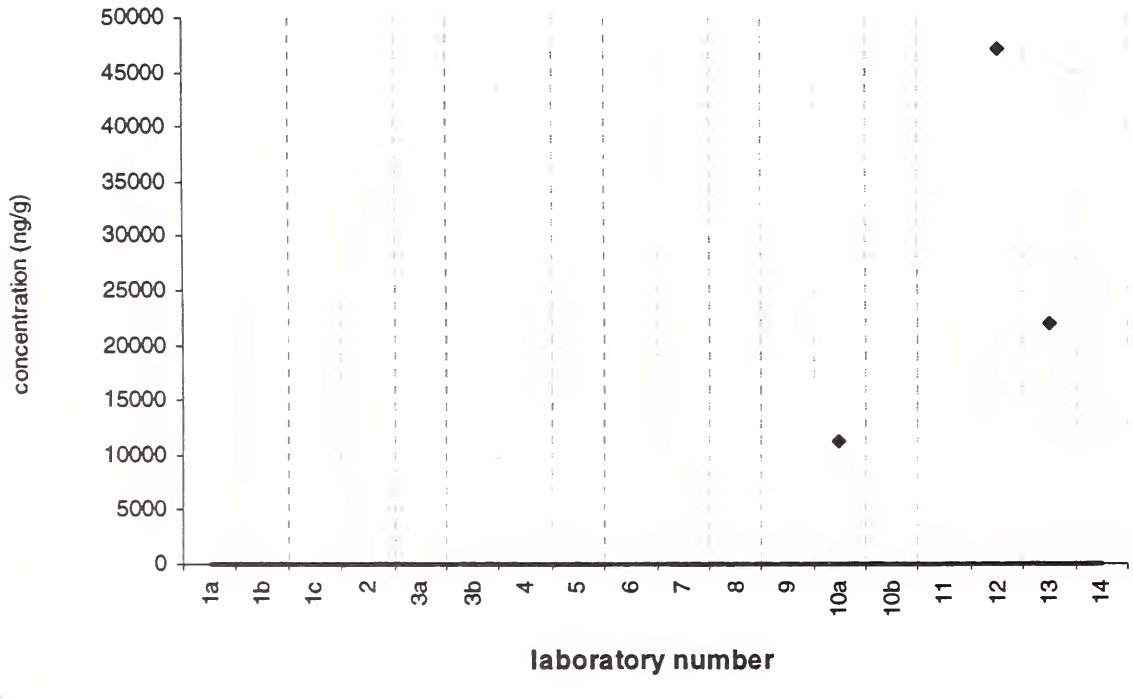


17a(H),21b(H)-Hopane (Chiron#0132,30)

SRM 1649a

Target Value = no target ng/g

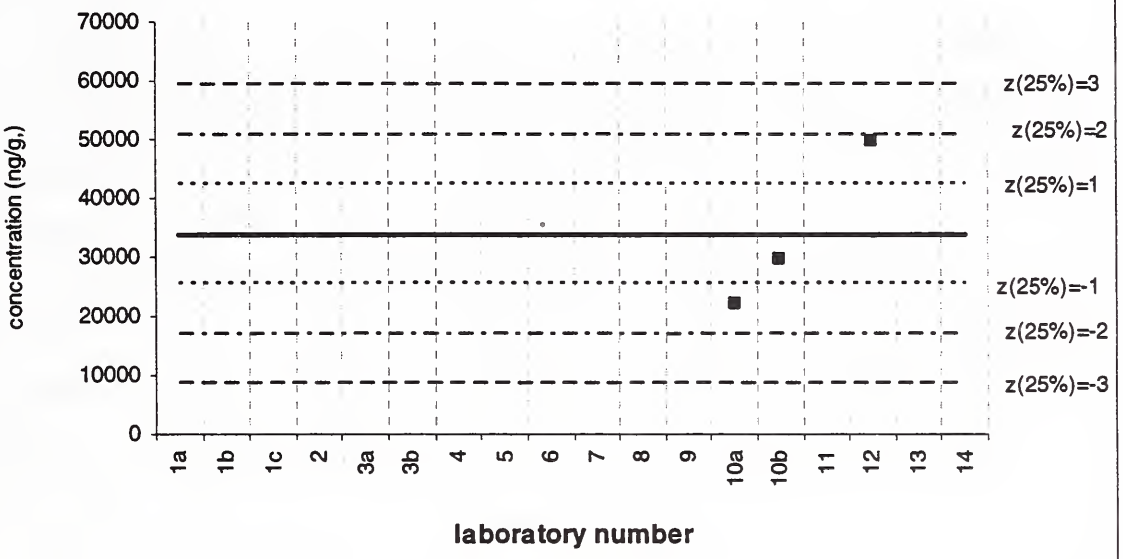
Reported Results: 3 Quantitative Results: 3



17a(H),21b(H)-Hopane (Chiron#0132,30) Filter samples

Assigned value (solid line) = 33871 ng/g s = 14165 ng/g 95% CL = 35188 ng/g

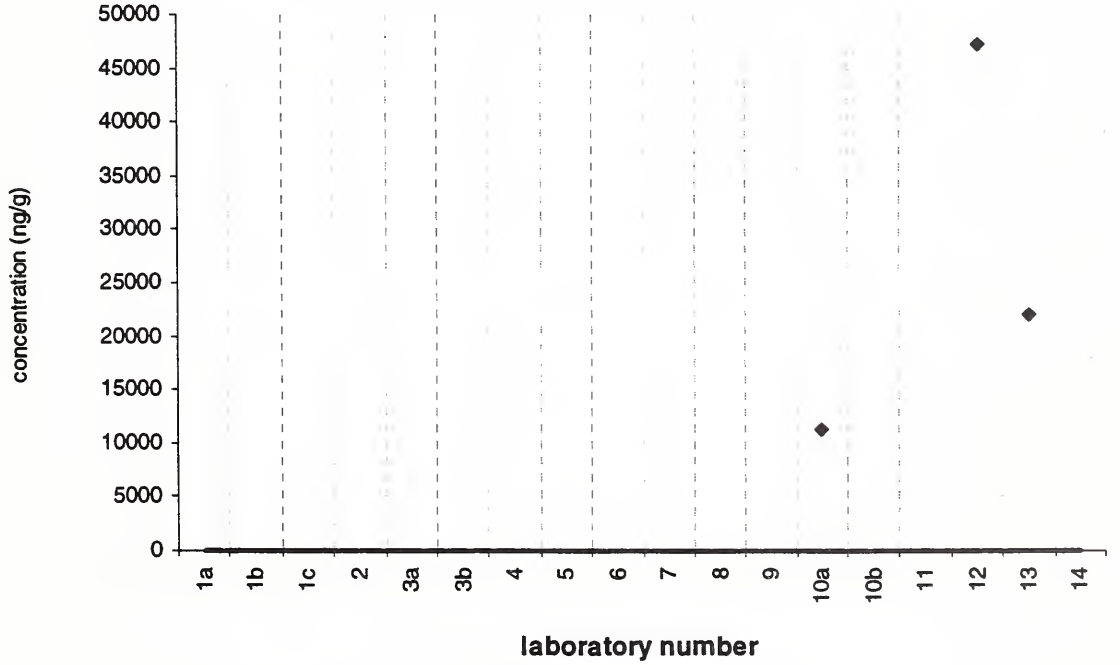
Reported Results: 3 Quantitative Results: 3



17a(H),21b(H)-Hopane (Chiron#0132,30) SRM 1649a

Target Value = no target ng/g

Reported Results: 3 Quantitative Results: 3

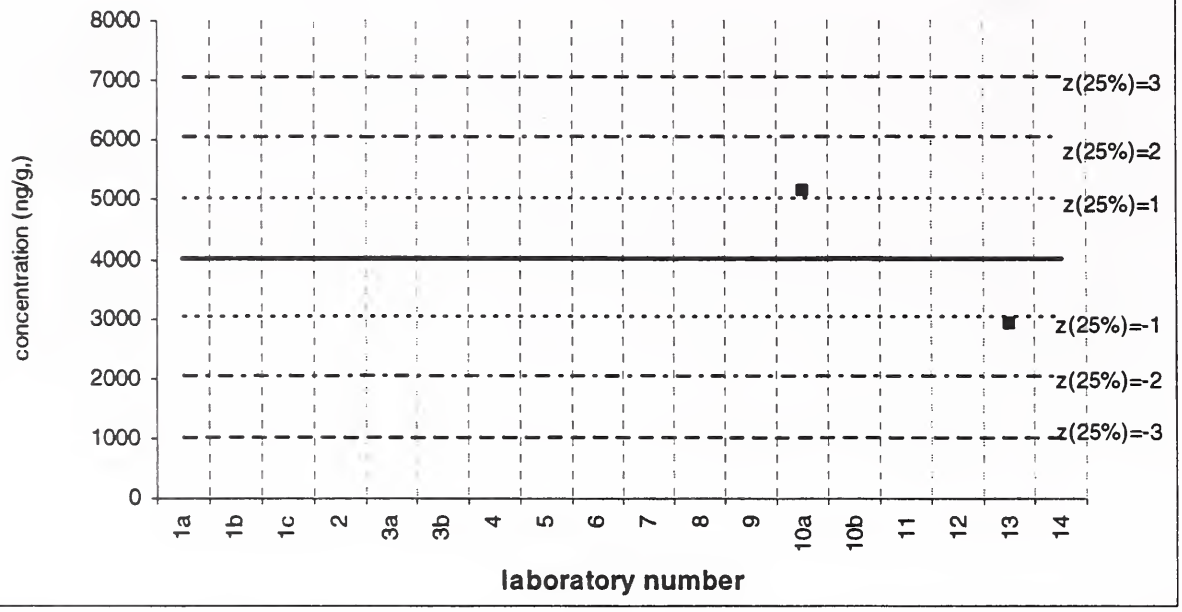


17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)

SRM 1648

Assigned value (solid line) = 4018 ng/g s = 1578 ng/g 95% CL = 14176 ng/g

Reported Results: 3 Quantitative Results: 2

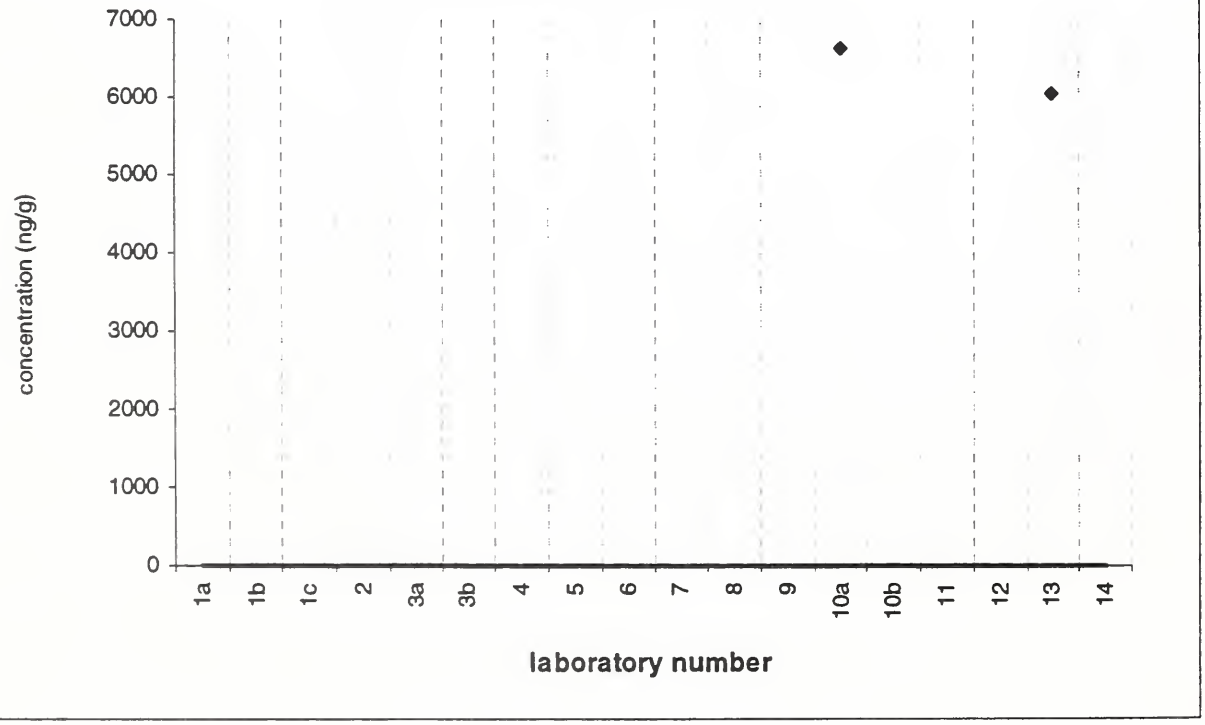


17a(H),21b(H)-22R-Homohopane (Chiron#1339,31)

SRM 1649a

Target Value = no target ng/g

Reported Results: 3 Quantitative Results: 2

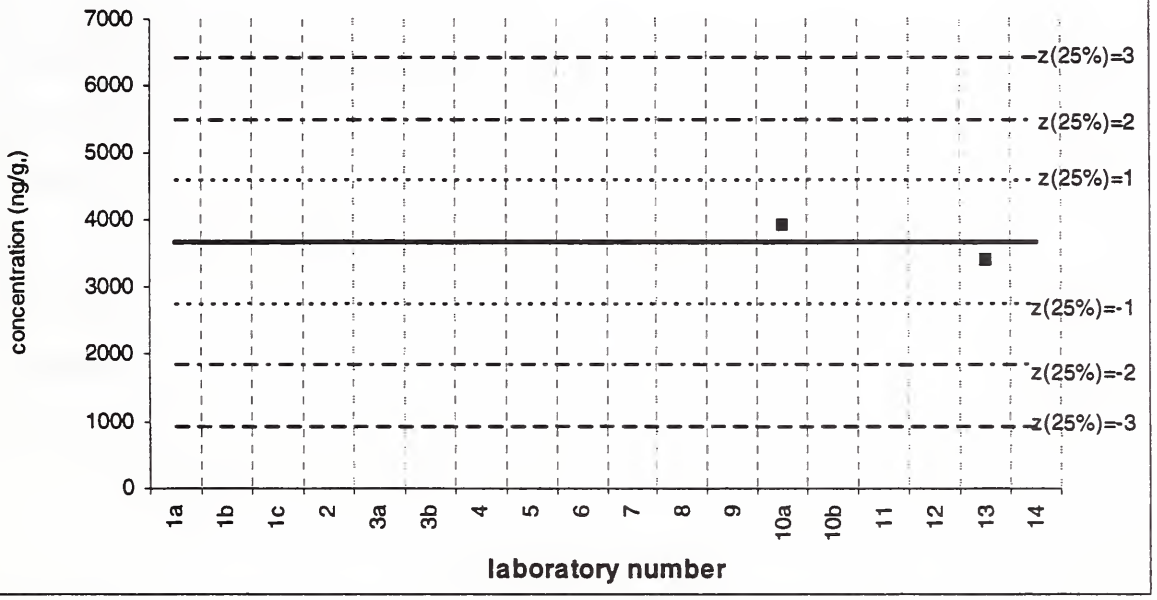


17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)

SRM 1648

Assigned value (solid line) = 3653 ng/g s = 349 ng/g 95% CL = 3138 ng/g

Reported Results: 3 Quantitative Results: 2

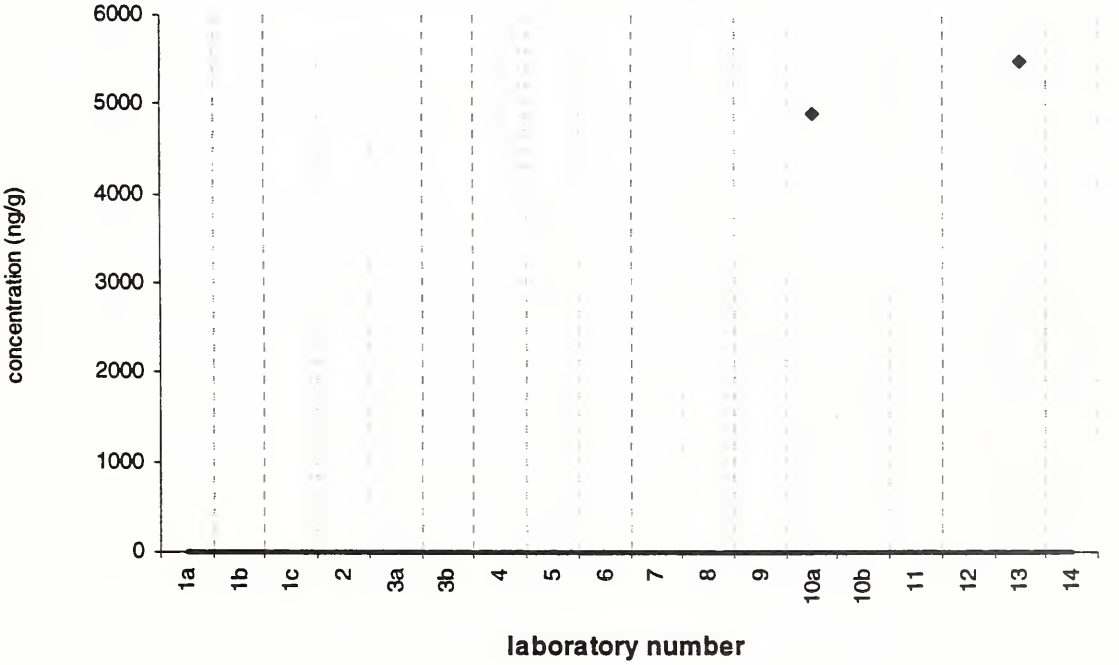


17a(H),21b(H)-22S-Homohopane (Chiron#1338,31)

SRM 1649a

Target Value = no target ng/g

Reported Results: 3 Quantitative Results: 2

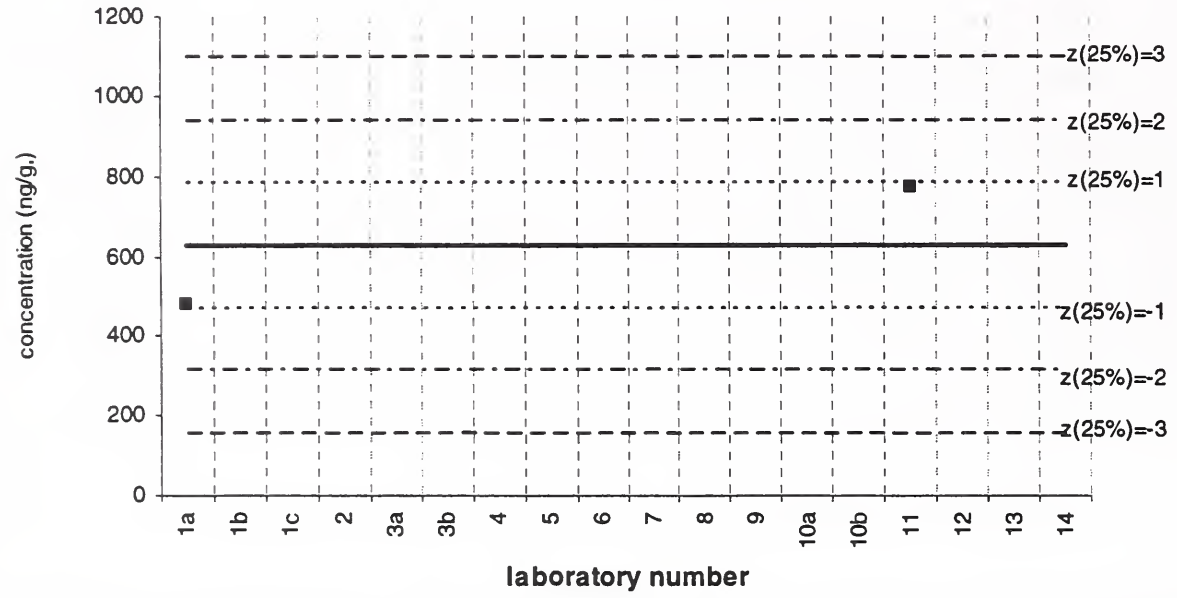


phytane

SRM 1648

Assigned value (solid line) = 626 ng/g s = 210 ng/g 95% CL = 1884 ng/g

Reported Results: 4 Quantitative Results: 2

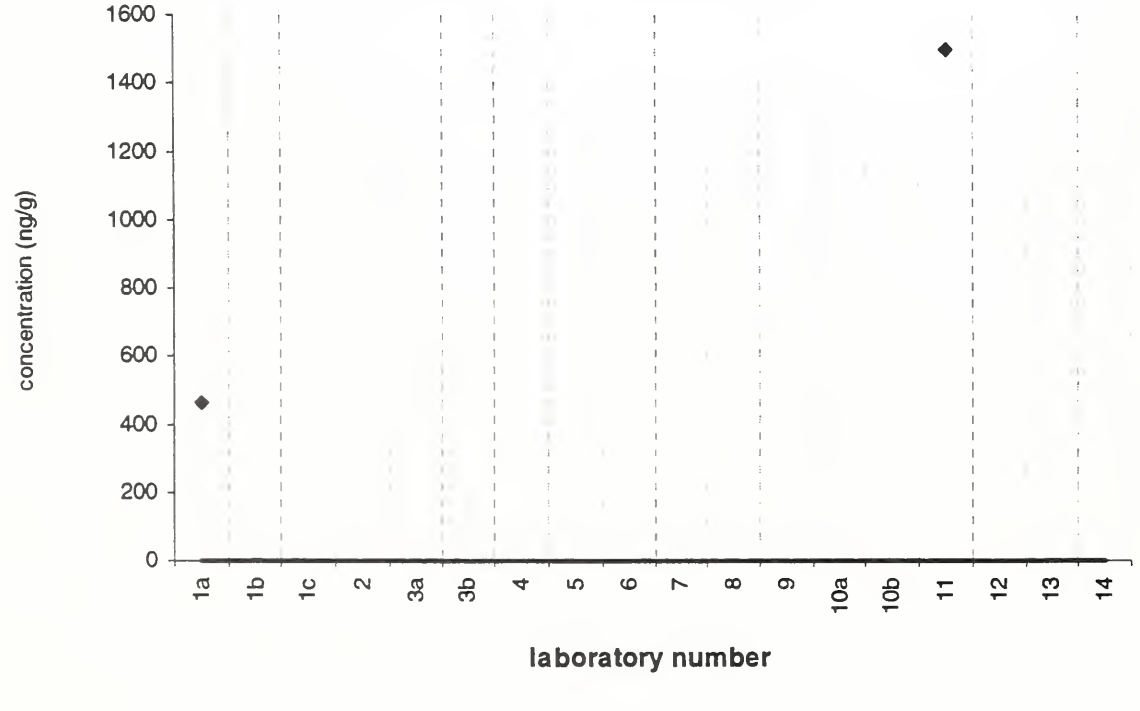


phytane

SRM 1649a

Target Value = no target ng/g

Reported Results: 4 Quantitative Results: 2

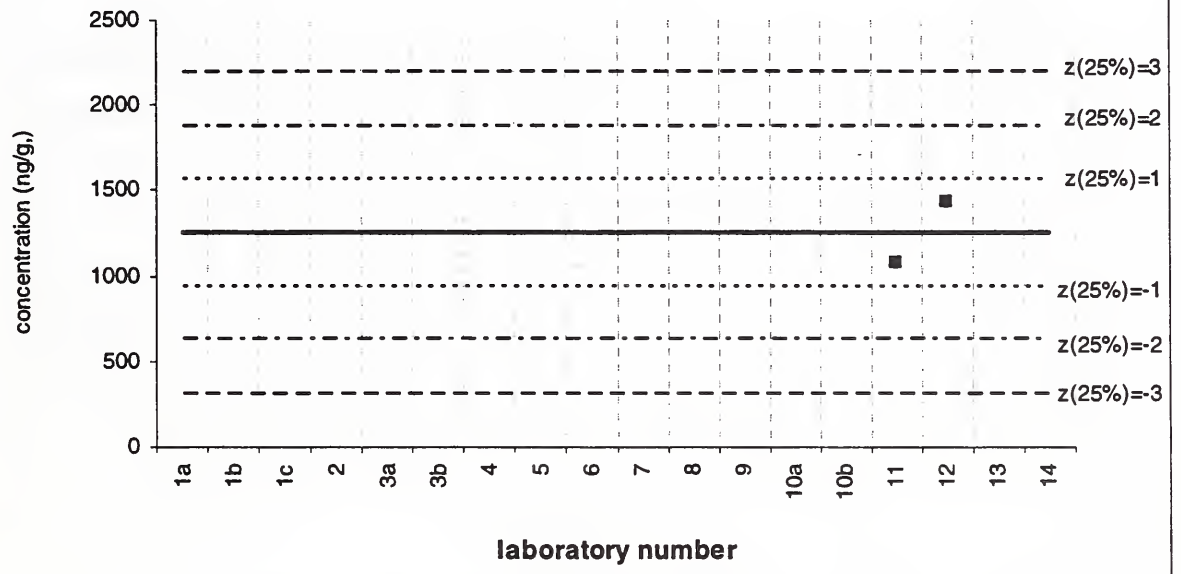


phytane

Baltimore 2 PM

Assigned value (solid line) = 1252 ng/g s = 250 ng/g 95% CL = 2249 ng/g

Reported Results: 4 Quantitative Results: 2

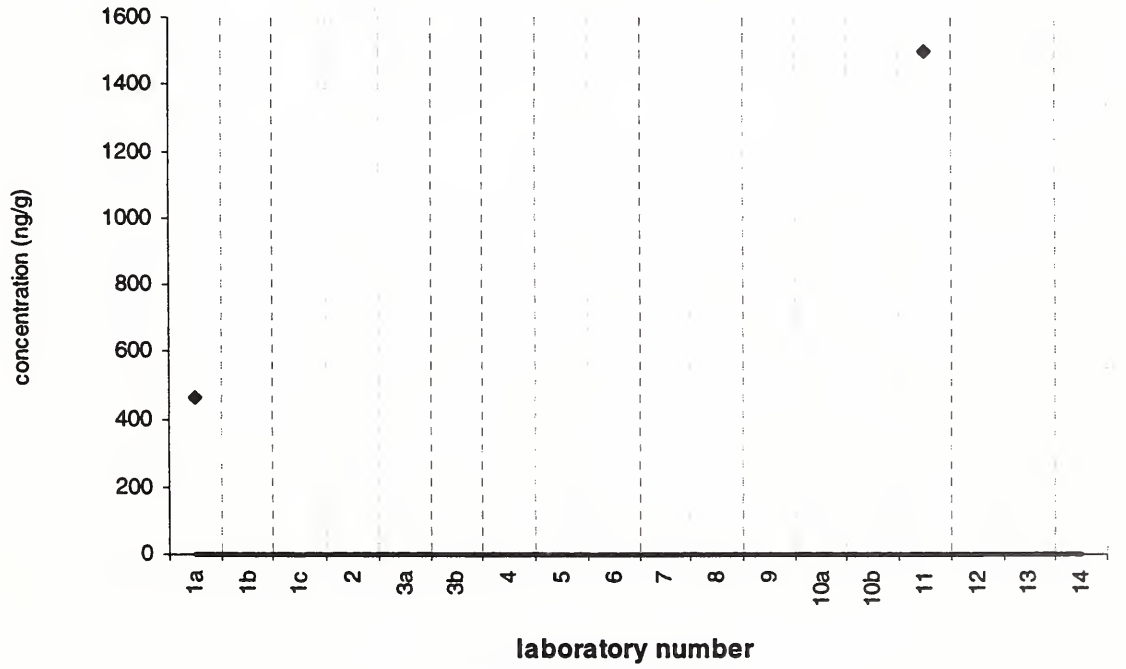


phytane

SRM 1649a

Target Value = no target ng/g

Reported Results: 4 Quantitative Results: 2

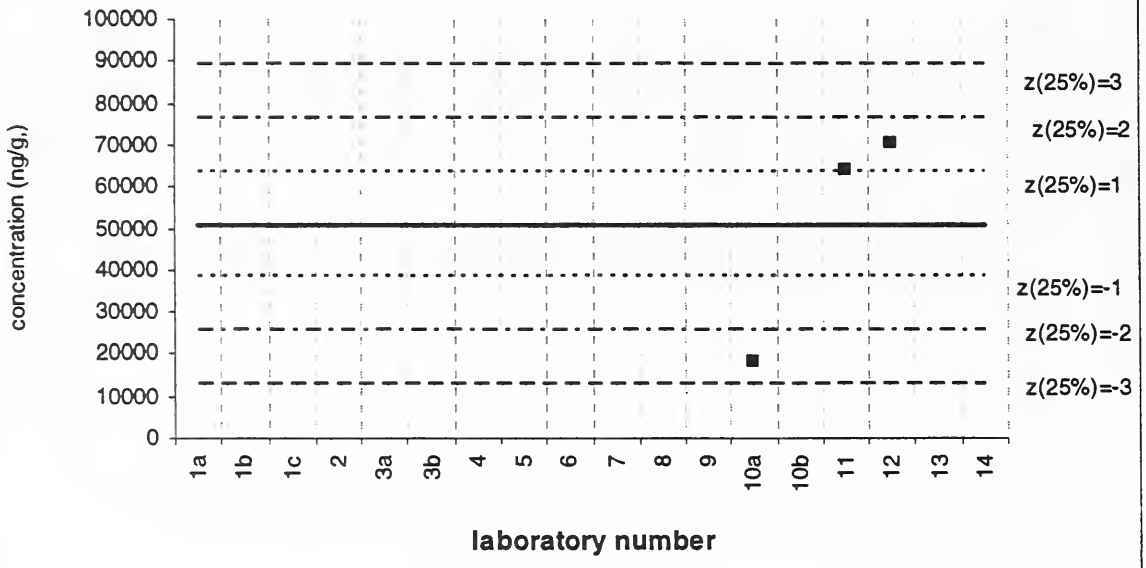


phytane

Filter samples

Assigned value (solid line) = 50983 ng/g s = 28435 ng/g 95% CL = 70636 ng/g

Reported Results: 3 Quantitative Results: 3

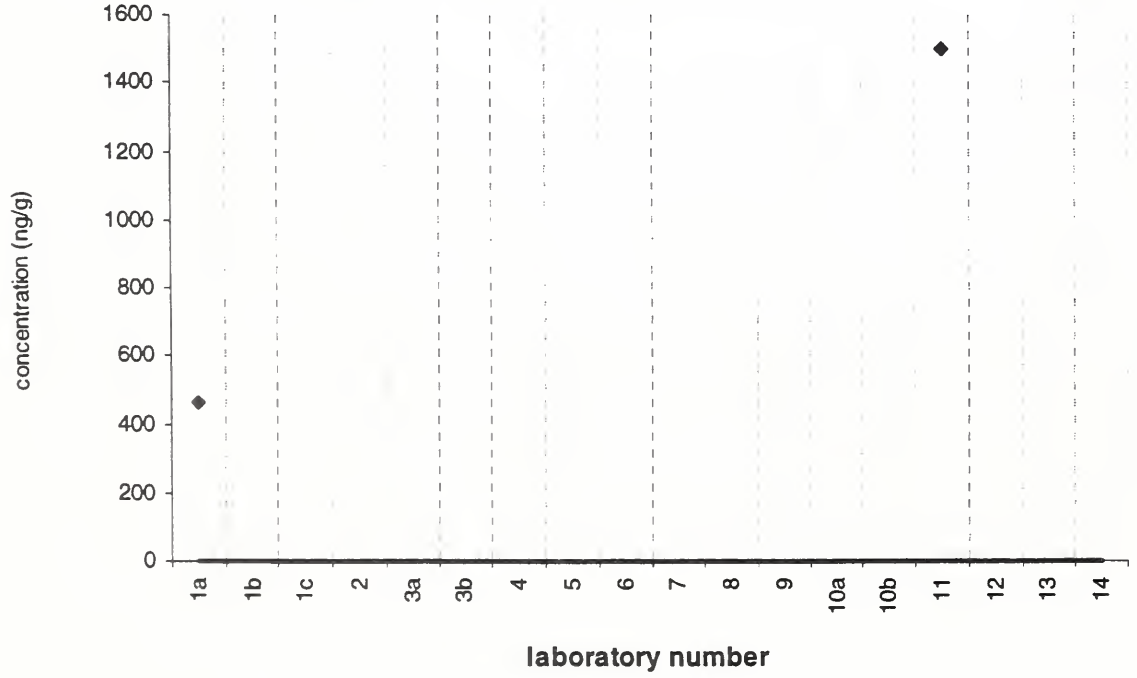


phytane

SRM 1649a

Target Value = no target ng/g

Reported Results: 4 Quantitative Results: 2

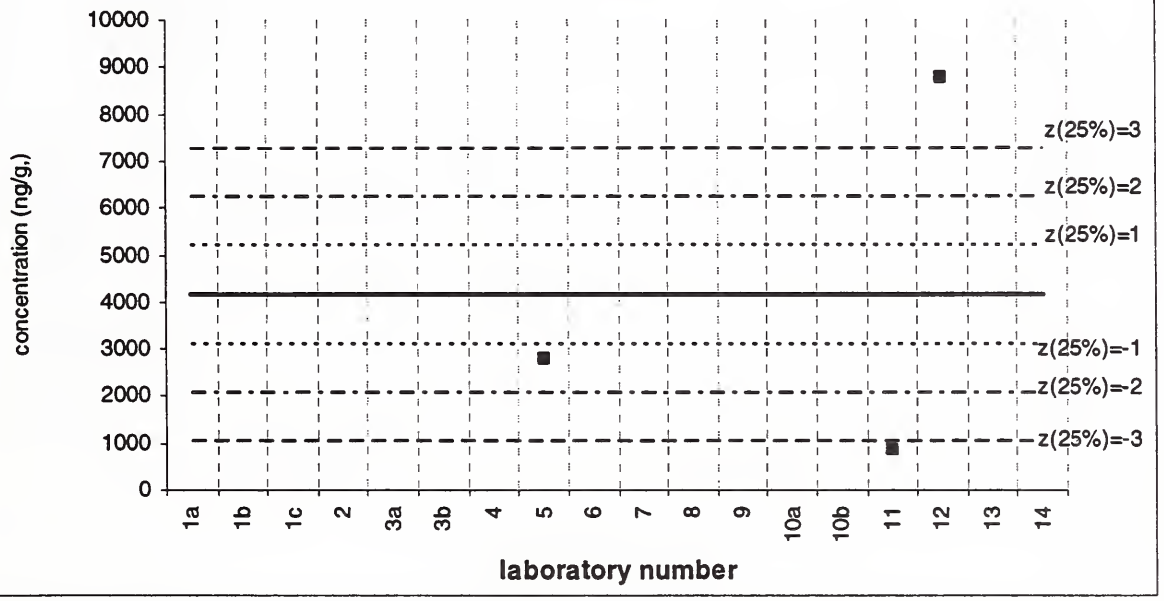


cholesterol

SRM 1648

Assigned value (solid line) = 4146 ng/g s = 4123 ng/g 95% CL = 10242 ng/g

Reported Results: 3 Quantitative Results: 3

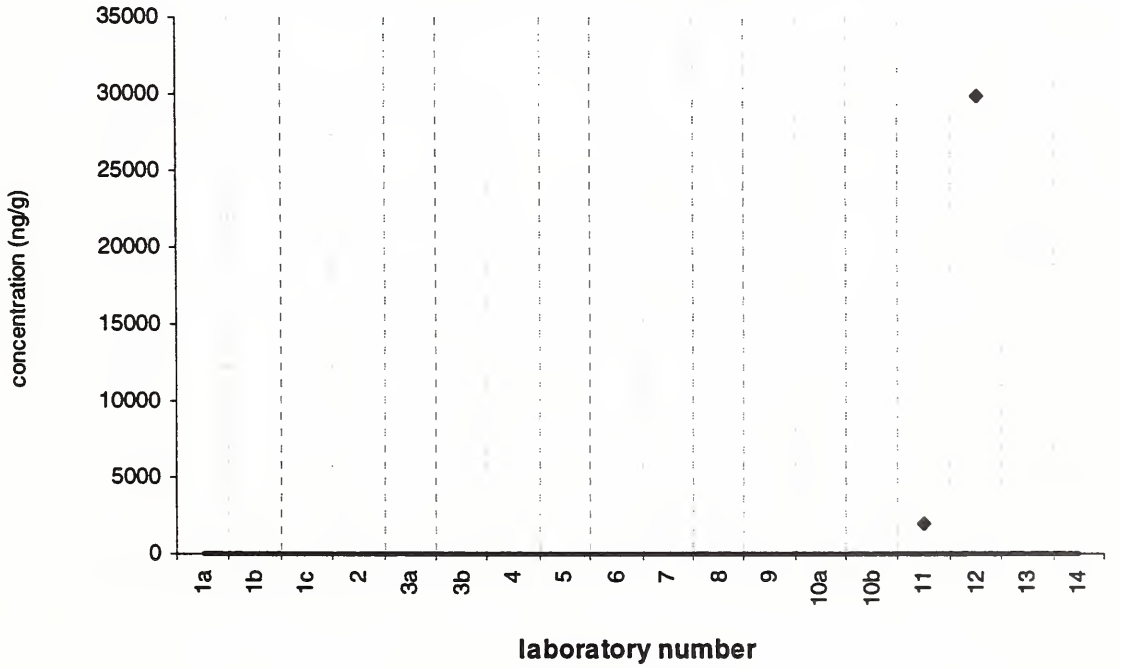


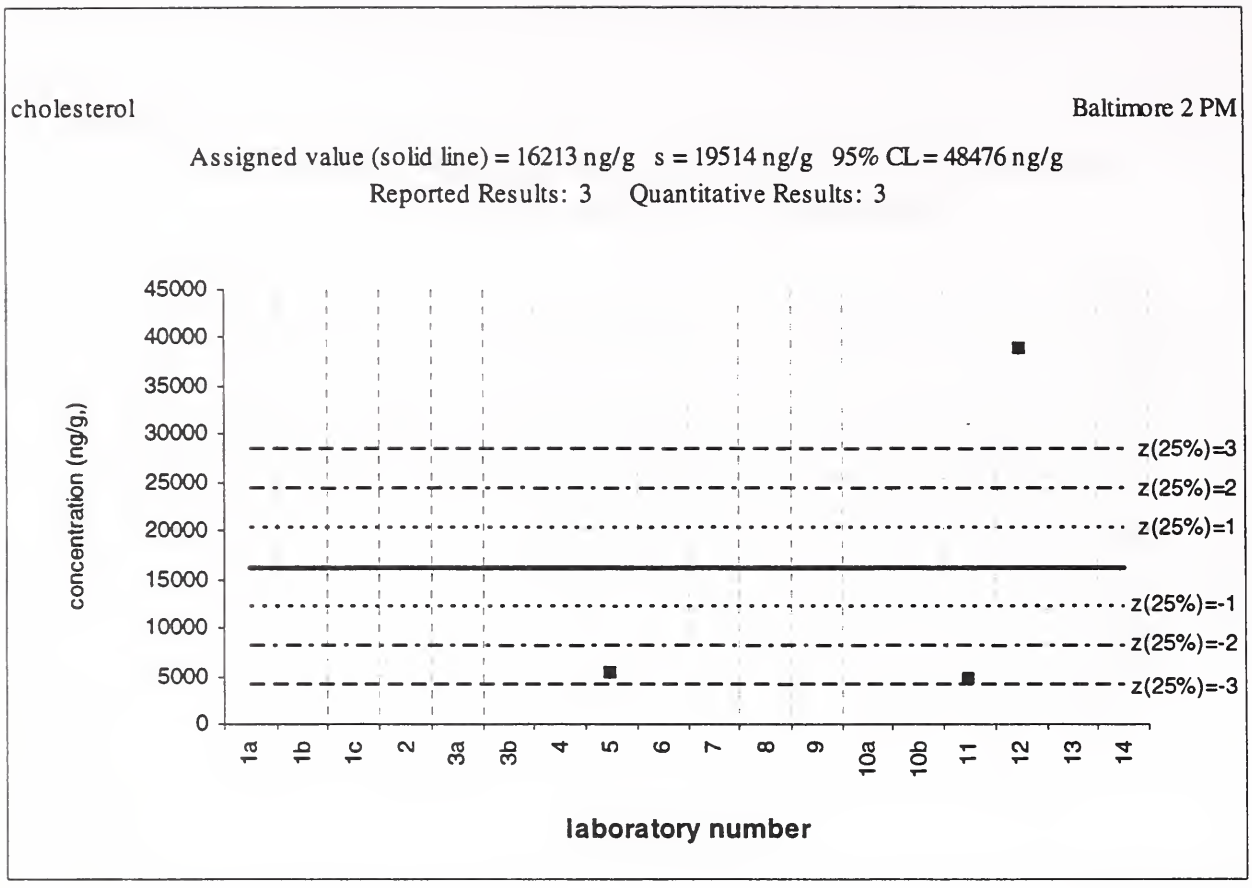
cholesterol

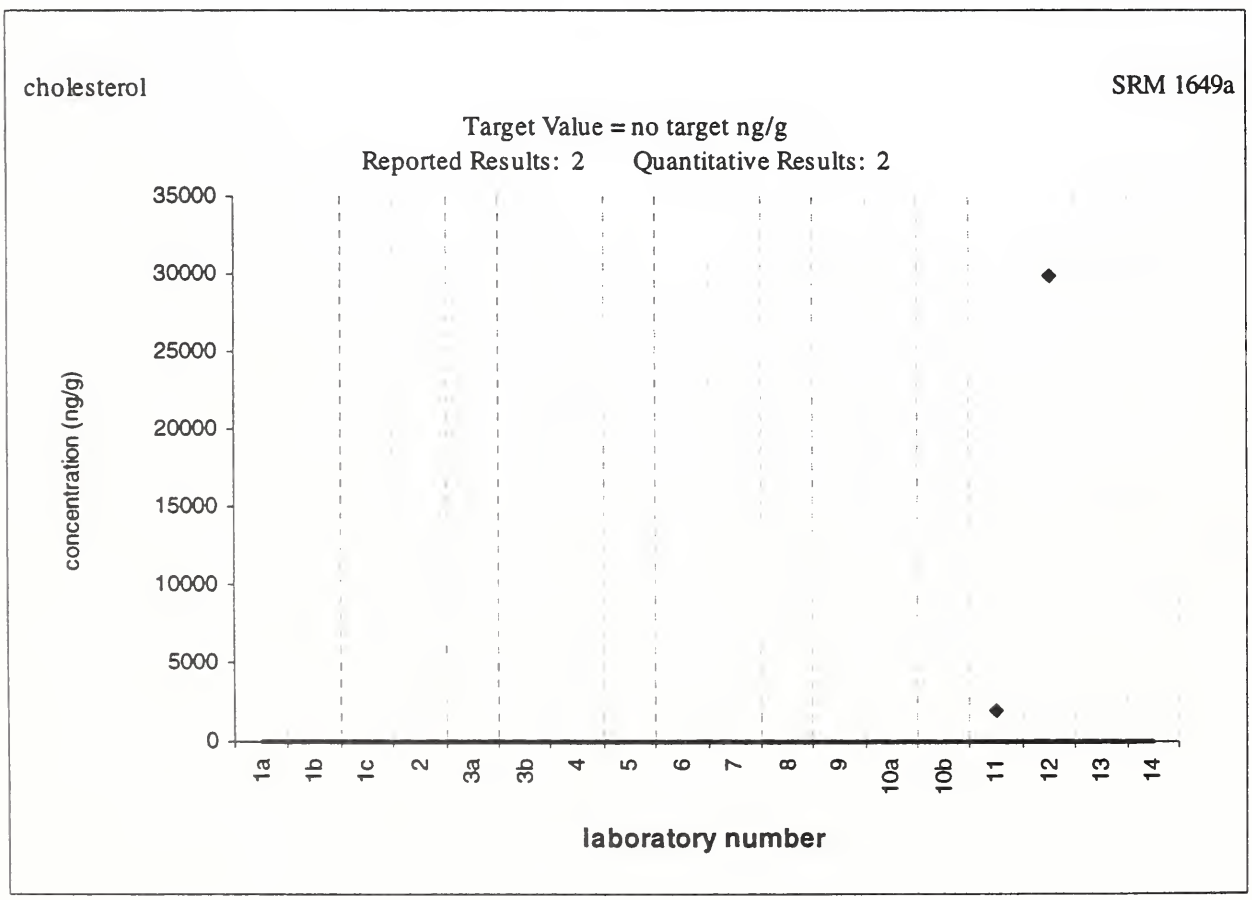
SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2




cholesterol
Baltimore 2 PM
Assigned value (solid line) = 16213 ng/g s = 19514 ng/g 95% CL = 48476 ng/g
Reported Results: 3 Quantitative Results: 3
concentration (ng/g)
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
z(25%)=3
z(25%)=2
z(25%)=1
z(25%)=-1
z(25%)=-2
z(25%)=-3
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

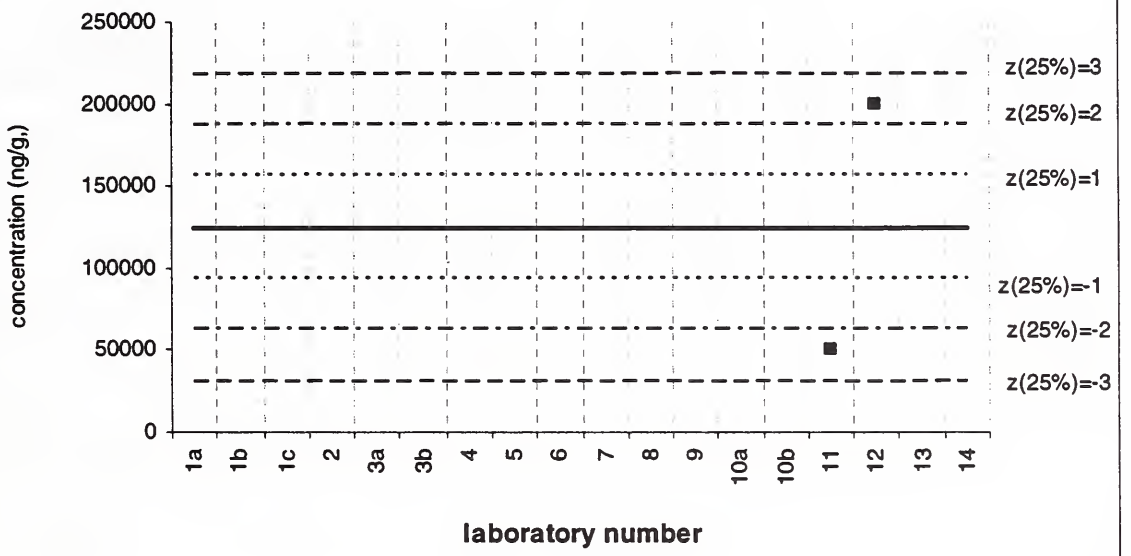

cholesterol
SRM 1649a
Target Value = no target ng/g
Reported Results: 2 Quantitative Results: 2
concentration (ng/g)
35000
30000
25000
20000
15000
10000
5000
0
1a
1b
1c
2
3a
3b
4
5
6
7
8
9
10a
10b
11
12
13
14
laboratory number

cholesterol

Filter samples

Assigned value (solid line) = 124752 ng/g s = 105172 ng/g 95% CL = 944926 ng/g

Reported Results: 2 Quantitative Results: 2

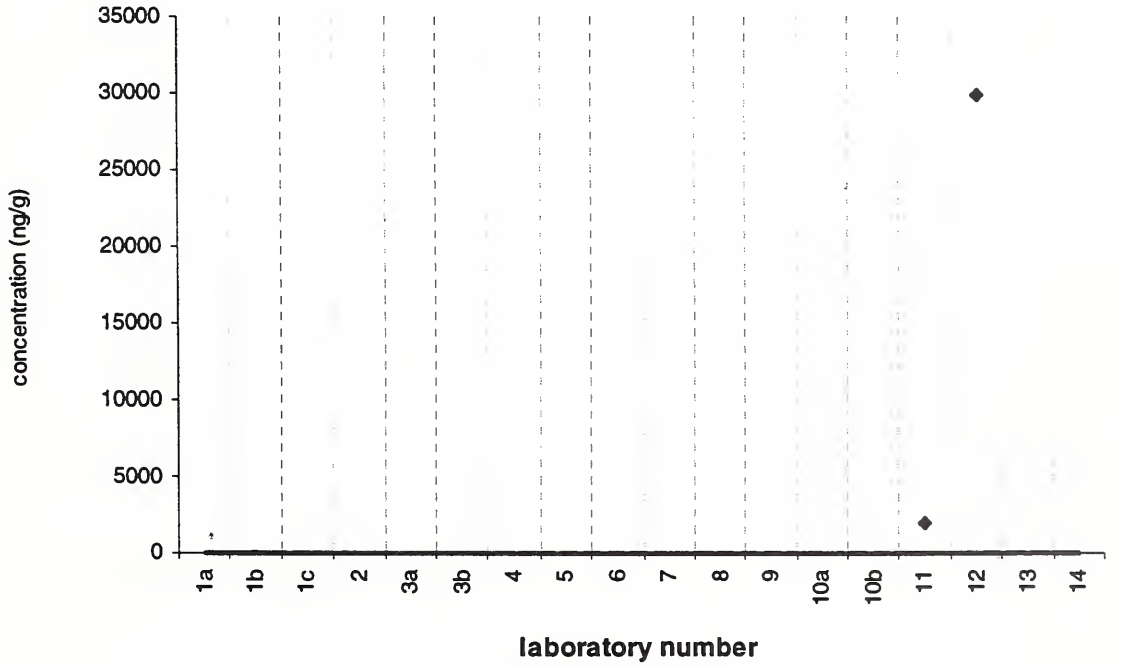


cholesterol

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

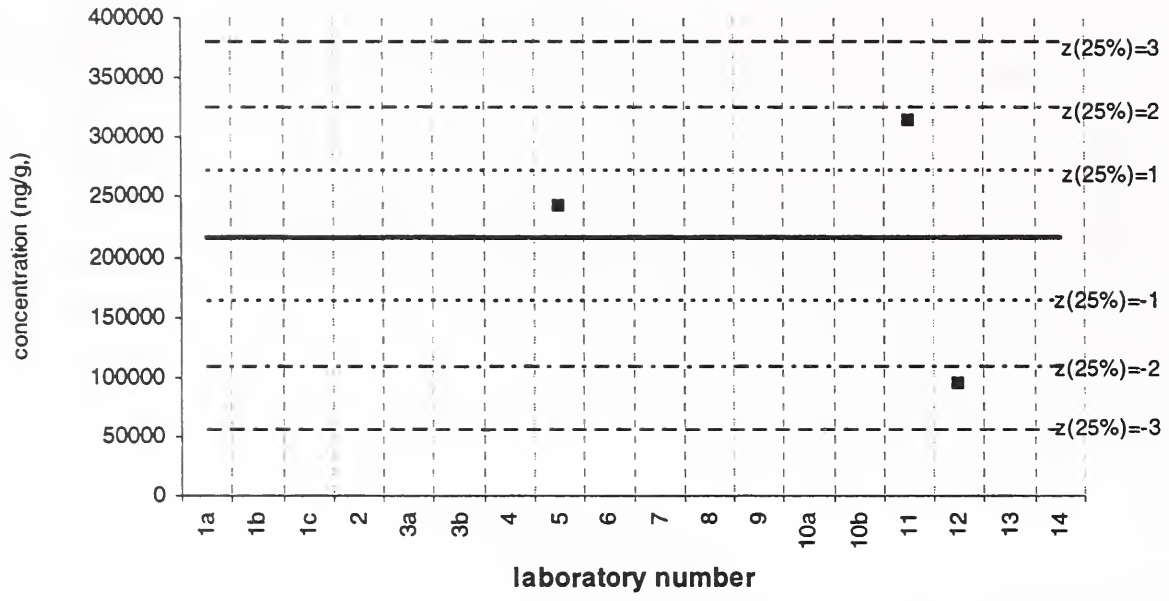


hexadecanoic acid

SRM 1648

Assigned value (solid line) = 216742 ng/g s = 112210 ng/g 95% CL = 278745 ng/g

Reported Results: 3 Quantitative Results: 3

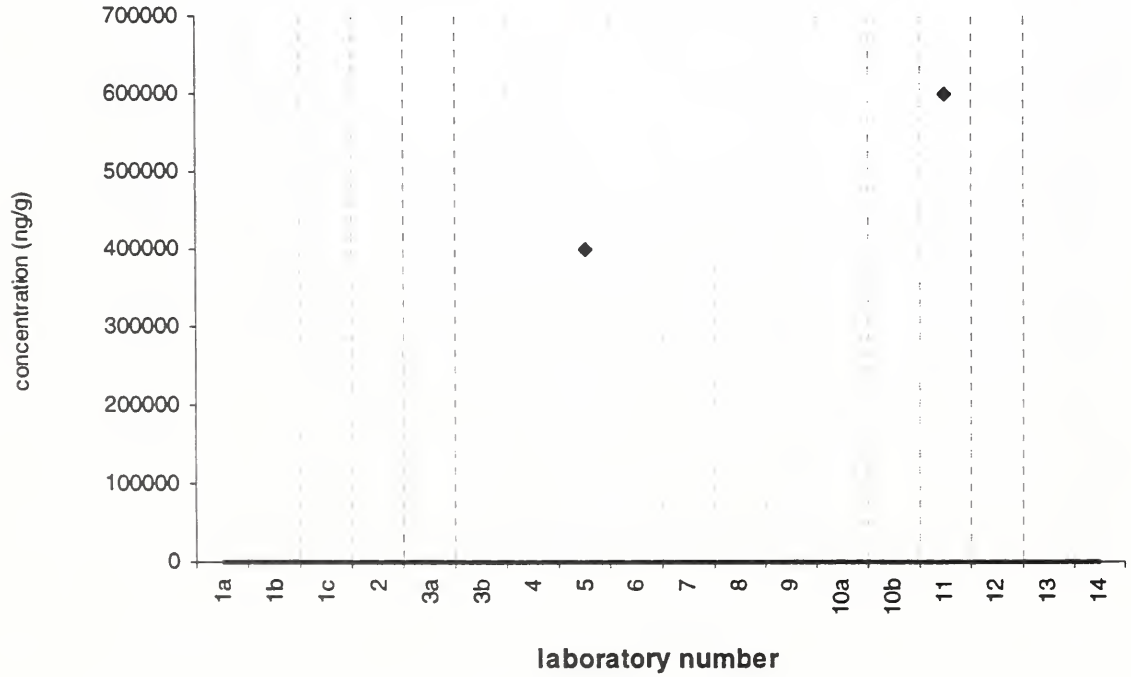


hexadecanoic acid

SRM 1649a

Target Value = no target ng/g

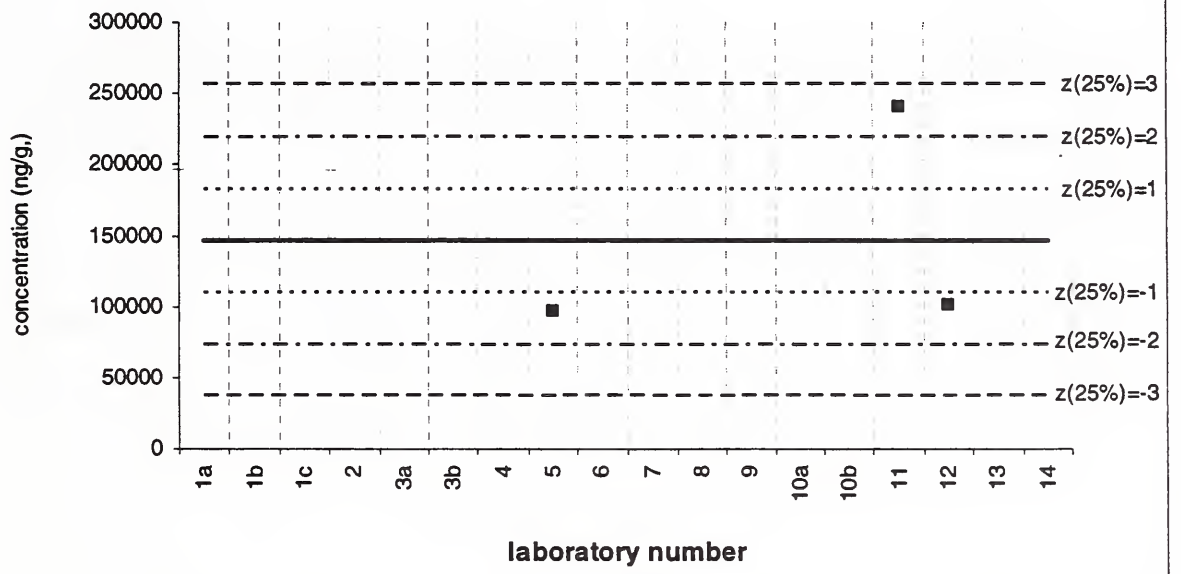
Reported Results: 2 Quantitative Results: 2



hexadecanoic acid Baltimore 2 PM

Assigned value (solid line) = 145987 ng/g s = 81945 ng/g 95% CL = 203563 ng/g

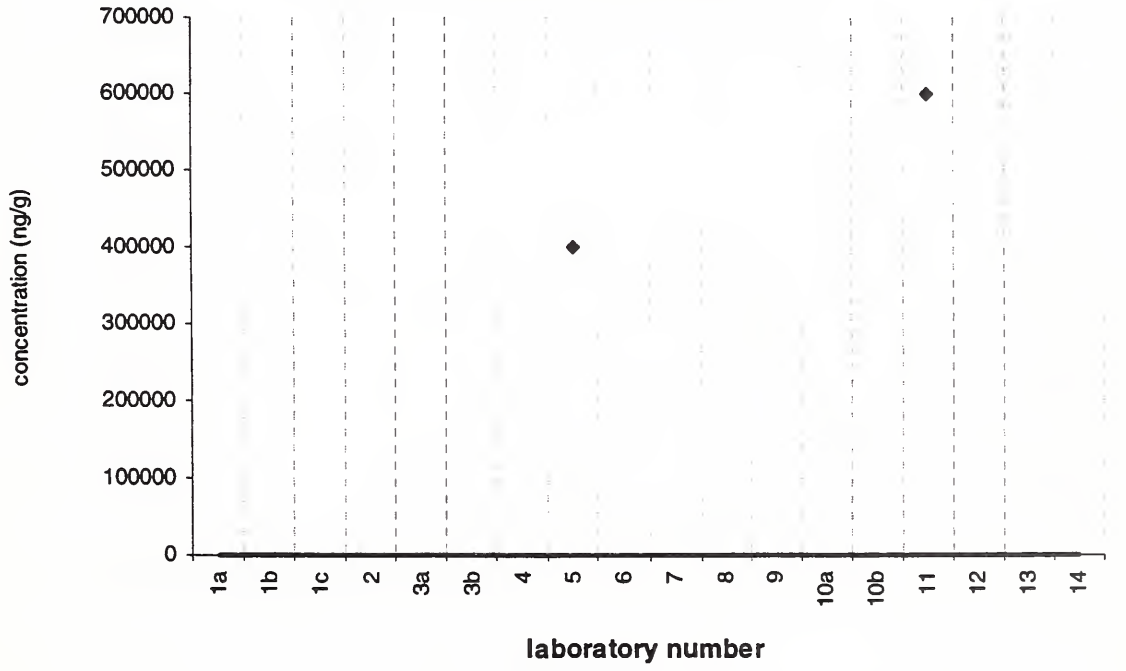
Reported Results: 3 Quantitative Results: 3



hexadecanoic acid SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

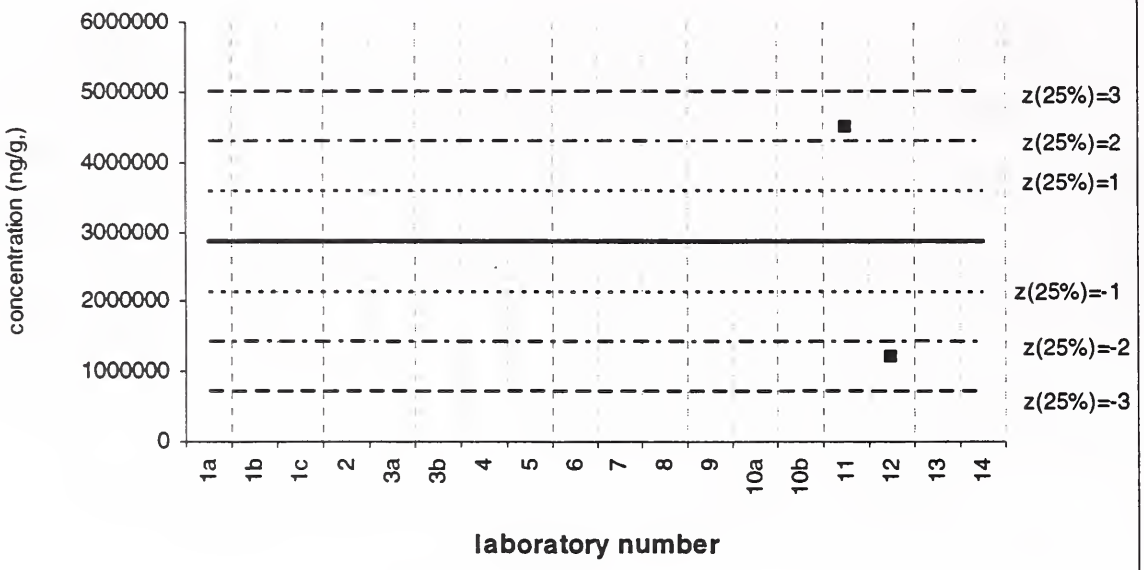


hexadecanoic acid

Filter samples

Assigned value (solid line) = 2855937 ng/g s = 2308061 ng/g 95% CL = 20737016 ng/g

Reported Results: 2 Quantitative Results: 2

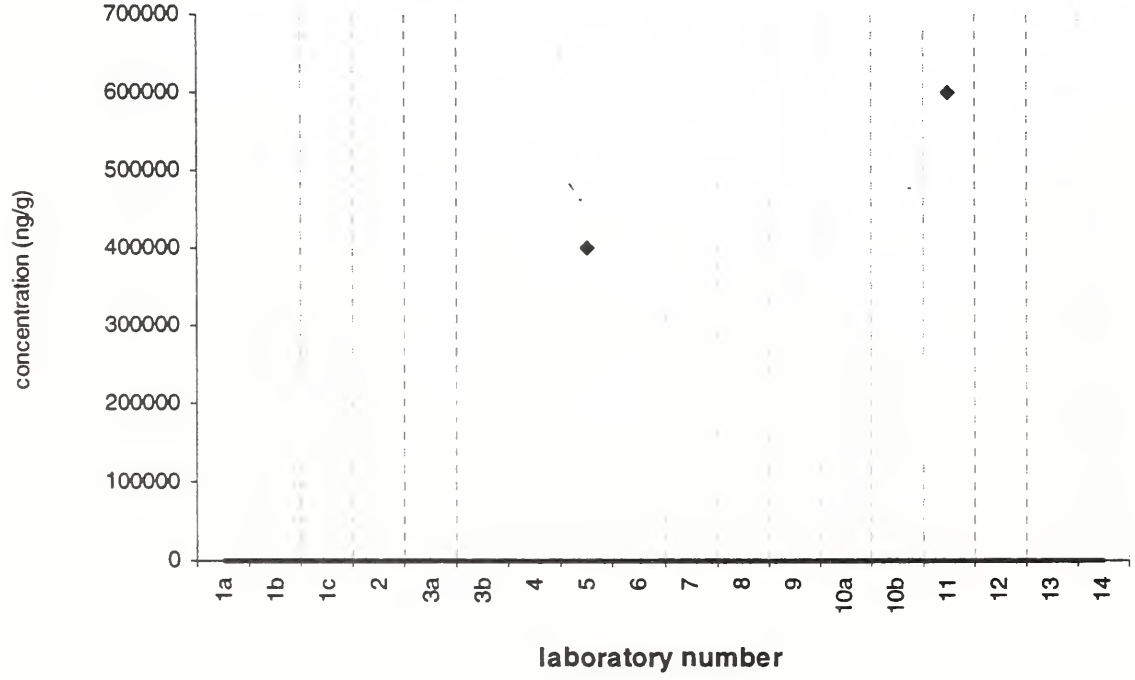


hexadecanoic acid

SRM 1649a

Target Value = no target ng/g

Reported Results: 2 Quantitative Results: 2

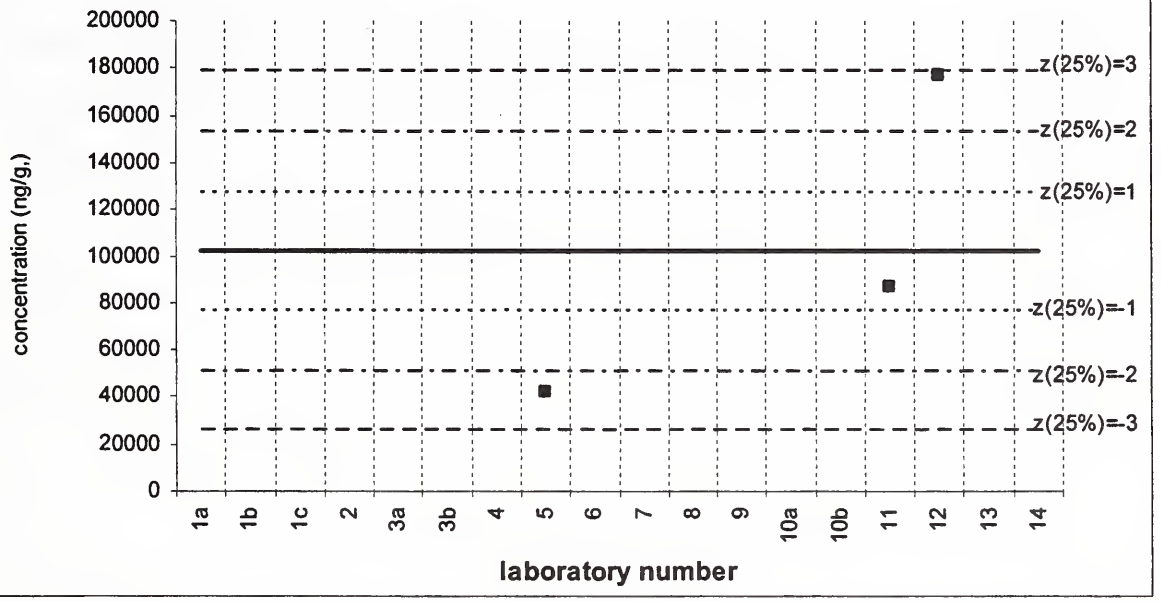


levoglucosan

SRM 1648

Assigned value (solid line) = 101947 ng/g s = 68612 ng/g 95% CL = 170443 ng/g

Reported Results: 3 Quantitative Results: 3

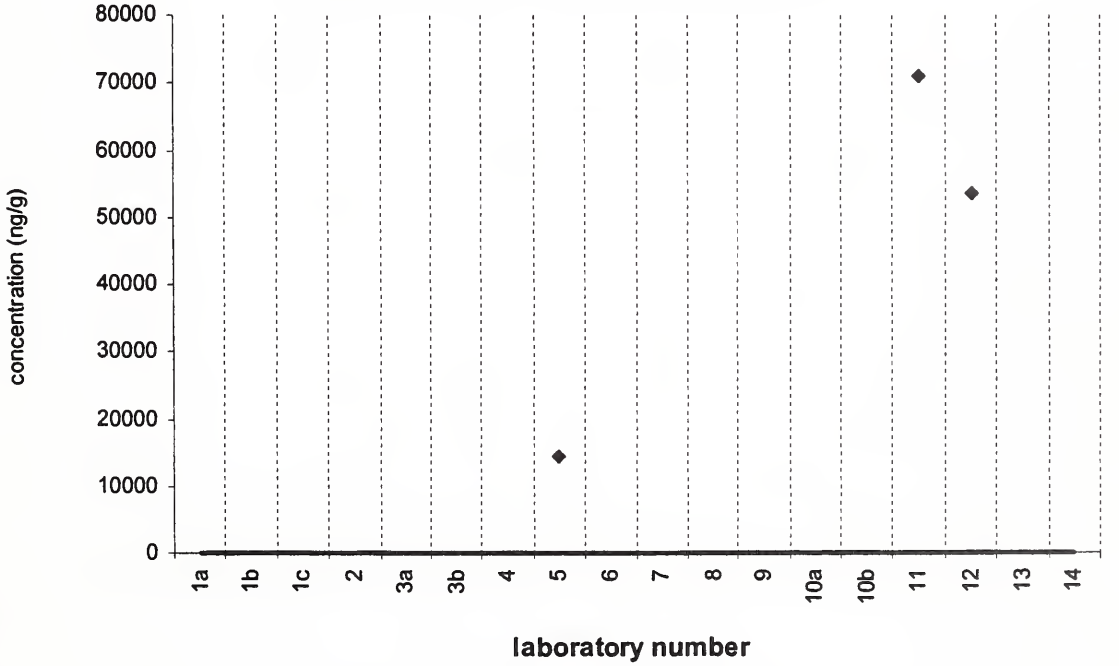


levoglucosan

SRM 1649a

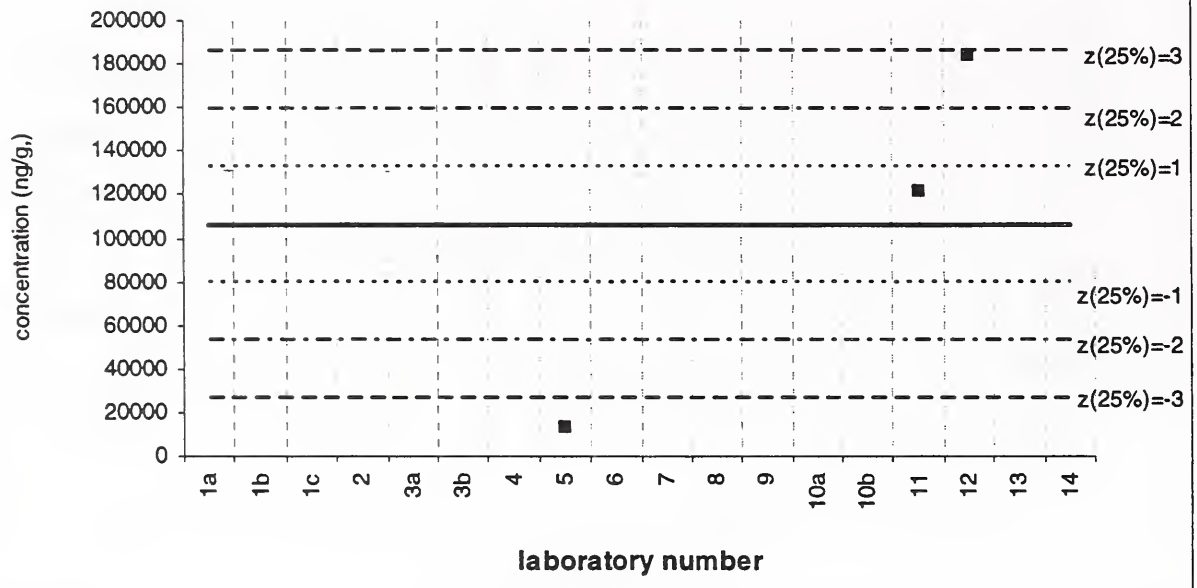
Target Value = no target ng/g

Reported Results: 3 Quantitative Results: 3



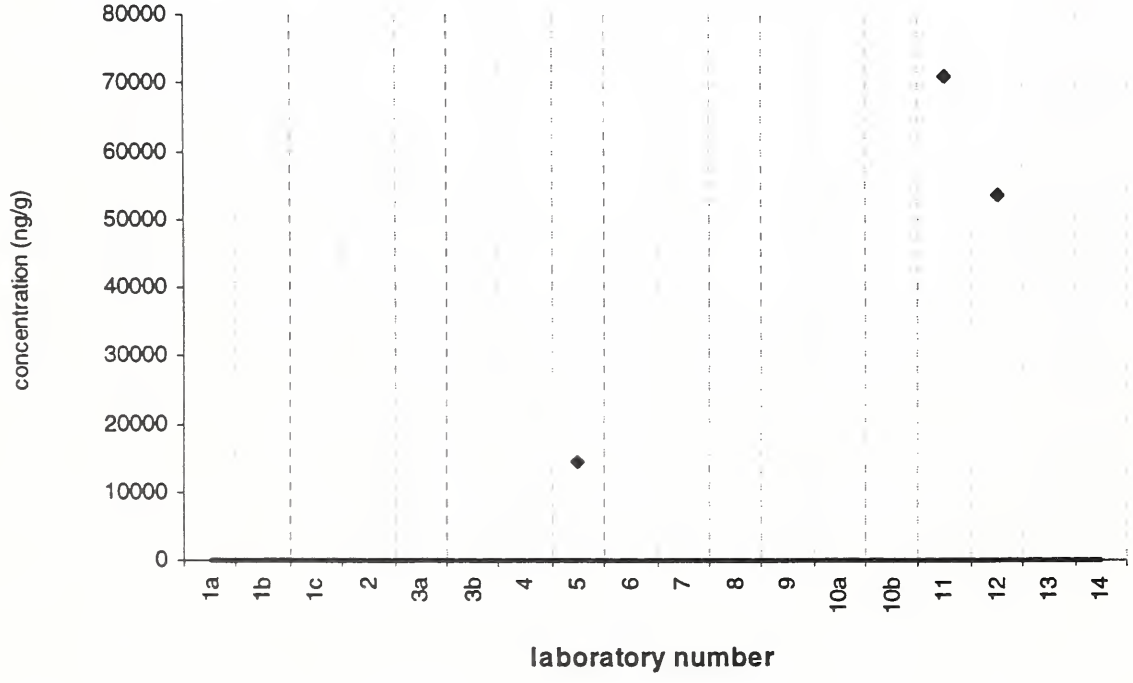
levoglucosan Baltimore 2 PM

Assigned value (solid line) = 106176 ng/g s = 86131 ng/g 95% CL = 213962 ng/g
Reported Results: 3 Quantitative Results: 3



levoglucosan SRM 1649a

Target Value = no target ng/g
Reported Results: 3 Quantitative Results: 3

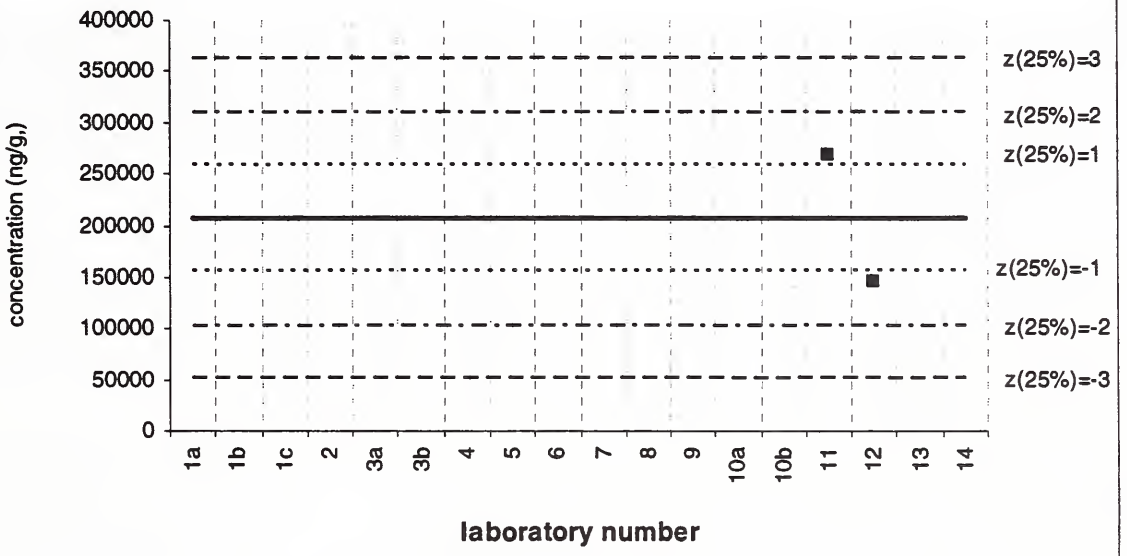


levoglucosan

Filter samples

Assigned value (solid line) = 206751 ng/g s = 85270 ng/g 95% CL = 766120 ng/g

Reported Results: 2 Quantitative Results: 2

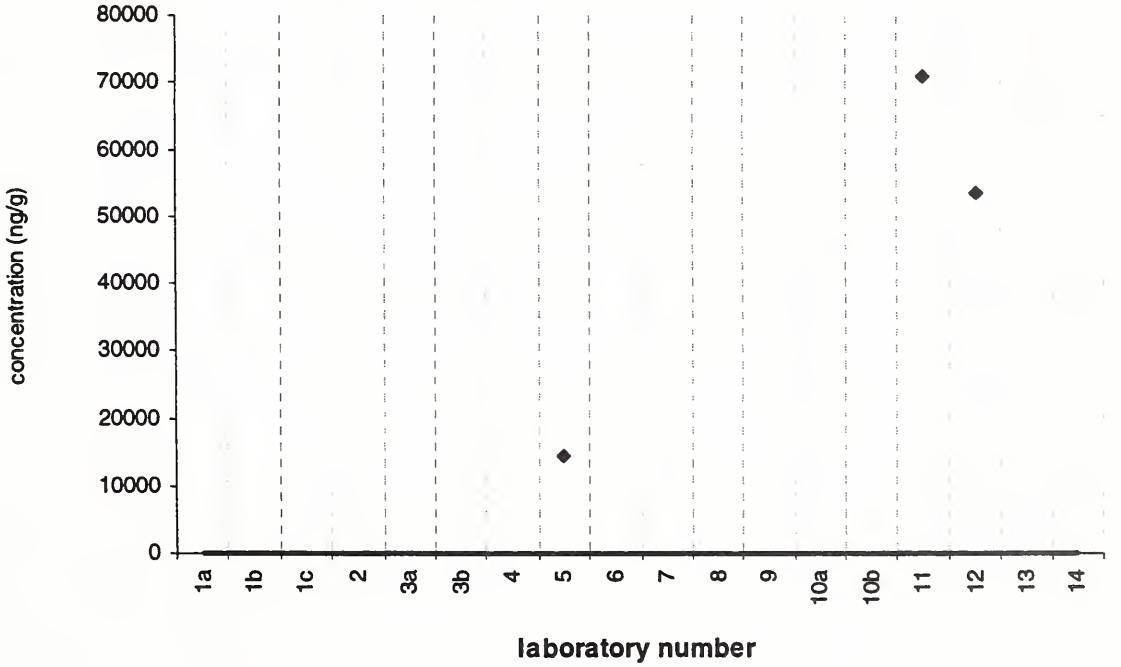


levoglucosan

SRM 1649a

Target Value = no target ng/g

Reported Results: 3 Quantitative Results: 3



Appendix E
List of Participants in Alphabetical Order by Institution

Arcadia
4915 Prospectus Drive
Suite F
Durham, NC 27713
Yuanji Dong / Mike Hays (EPA – RTP)

Centro de Ciencias de la Atmósfera
Universidad Nacional Autónoma de México
Ciudad Universitaria, Coyoacán 04510
D.F., México
M. en C. Omar Amador Muñoz/ Rafael Villalobos Pietrini

Desert Research Institute
2215 Raggio Parkway
Reno, NV 89512
Barbara Zielinska / Lynn Rinehart

Ecochem a.s.
Dolejškova 3
Prague 8, Czechoslovakia – 182 00
Ing. Rudolf Gomola; Mgr. Alena Housová

Environment Canada
Analysis and Air Quality Division
335 River Road South
Golucester, Ontario K1V 1C7 Canada
Chung Chiu / Gary Poole

Environment Canada
Atmospheric Research Directorate Processes Research Division (ARQP) /
Meteorological Service of Canada
4905 Dufferin Street
Downsview, Ontario M3H 5T4 Canada
Amy Leithead / Shao-Meng Li / Yu Cheng

Finnish Institute of Occupational Health
Chemistry Laboratory
Topeluksenkatu 41 aA
00250 Helsinki Finland
Kirsti Savela

GSF – National Research Center for Environment and Health
Ingolstaedter Landstrasse 1
D-85764 Oberschleissheim, Germany
Georg Matuschek

ISPESL/DIPIA
Via di Fontana Candida, 1
00040 Monteporzio Cantone, ROMA Italy
Patrizia Di Filippo

IST- Institute of Occupational Health Sciences
19 Rue du Bugnon
Ch-1005 Lausanne Switerland
Huynh Cong Khanh

Natural Resources Canada
1 Haanel Drive
Ottawa, Ontario K1A 1M1
Jean-Pierre Charland / Pamela (Penny) MacDonald

NIST
100 Bureau Dr, Stop 8392
Gaithersburg, MD 20899-8392
Michele Schantz / Dianne Poster

NIST
Hollings Marine Laboratory
331 Fort Johnson Rd
Charleston, SC 29412
John Kucklick

Rutgers University
Department of Civil and Environmental Engineering
623 Bowser Rd
Piscataway, NJ 08854
Monica Mazurek

Southern California Particle Center and Supersite
650 Charles E. Young Dr
South ((PMCAL)-51.297 CHS)
Los Angeles, CA 90095-1772
Toni Miguel / Arantra Eiguren-Fernandez